Electronic Supplementary Material (ESI) for RSC Advances

Electronic Supporting Information

How Do Perfluorinated Alkanoic Acids Elicit Cytochrome P450 to Catalyze Methane Hydroxylation? An MD and QM/MM Study

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Abbreviations:

SnapX1: snapshot after 1823 ps of production.

SnapX2: snapshot after 1ns of production.

B1: LACVP

B2: LACV3P++**

B3: def2-TZVP

B4: LACV3P+*

1. Protonation scheme:

The resid of the protonated Glu: 4, 13, 35, 140, 252, 348, 373, 409

The resid of the protonated Asp: 199, 222, 231, 251, 369

The resid of the histidines protonated only at δ-N atom (HSD): 92, 100, 116, 171, 236, 266, 361, 408, 420, 426

The resid of the histidines protonated only at ε-N atom (HSE): 388

The resid of the histidines protonated at both ε- and δ-N atom (HSP): 138, 285.

2. Active region in QM/MM calculation:

ARG47 THR49 LYS69 SER72 GLN73 ALA74 LEU75 VAL78 PHE81 ALA82 LEU86 PHE87 TRP96 HSD100 PHE107 ILE153 LEU181 LEU188 LEU233 THR260 PHE261 ILE263 ALA264 GLY265 GLU267 THR268 THR269 LEU272 LEU322 THR327 ALA328 PRO329 ALA330 PHE331 SER332 GLU352 MET354 ILE357 PRO392 PHE393 GLY394 ARG398 ALA399 ILE401 GLY402 GLN403 PHE405 ALA406 LEU437 THR438 HEC2 PFDA METH3 CRYW501 CRYW504 CRYW510 CRYW515 CRYW521 CRYW537 CRYW544 CRYW548 CRYW749 CRYW983 CRYW1037 CRYW1275 SOLV33 SOLV40 SOLV313 SOLV380 SOLV794 SOLV2913 SOLV3233 SOLV3245 SOLV3268 SOLV3461 SOLV3617

3. Force field:

The topology and parameter files of Cpd I are taken from previous study.[1] The PFDA is not among the predefined residues of the CHARMM library. It was treated as follows:

(1) B3LYP/6-31G* optimization on PFDA ($C_9F_{19}COOH$) by G09;

(2) B3LYP/6-31G* optimization on decanoic acid (DECA, $C_9H_{19}COOH$) by G09;

(3) Assigned the atom types of PFDA and DECA according to CHARMM conventions;

(4) Utilized PARATOOL embedded in VMD[2] to generate topologies and parameters of PFDA and DECA;

(5) The CHARMM atom types of DECA are CT3, CT2, CD, HA, OB, OH1, H and their related parameters can be found in CHARMM standard parameter library. According to the DECA's CHARMM standard parameters, we assigned the final parameters of PFDA by comparing the parameters of PFDA and DECA generated from step 4.

(6) The charges of PFDA were chosen in analogy to CHARMM whenever possible and were derived by referring to CGenFF[3] library.

(7) The resulting parameter set for PFDA was validated by the following set of calculations:

(7-1). A water layer of 35 angstroms thickness was constructed around PFDA.

(7-2). 200 steps of SD minimization and 1000 steps of ABNR minimization by CHARMM.

(7-3). 30ps heating dynamics to 300K, 50 ps equilibration and 200 ps production by

CHARMM.

During the above MD running, the outer 10 angstrom water layer was kept fixed. The RMSD of PFDA between the final CHARMM production structure and the G09 optimized structure is 0.46. The MD results are summarized in Table S1.

Table S1. Representative Bond length (angstrom), angle (degree) and improper torsion angle (degree) in PFDA during MD running.

	G09 B3LYP/6-31G* optimization	CHARMM Optimization	CHARMM 200 ps production		
			Minimum	Maximum	RMS
C29-F32	1.338	1.339	1.263	1.412	0.03
C26-F27	1.351	1.357	1.293	1.429	0.02
C17-F18	1.353	1.356	1.284	1.436	0.03
C5-F7	1.356	1.355	1.293	1.426	0.03
C1-O2	1.201	1.205	1.157	1.256	0.02
C1-O3	1.341	1.357	1.248	1.429	0.03
O3-H4	0.977	0.977	0.977	0.978	0.00
F32-C29-C26	110.3	110.3	105.0	118.5	2.11
C29-C26-C23	114.2	115.0	109.8	120.1	1.93
C23-C20-C17	113.3	114.1	109.1	118.9	1.72
C1-C5-C8	112.3	112.2	106.4	117.8	2.12
F15-C14-F16	109.3	108.4	101.7	116.3	2.47
O3-C1-O2	126.2	123.0	118.4	131.4	2.13
O2-C1-C5	123.5	123.4	116.3	128.6	2.18
O3-C1-C5	110.3	113.5	105.9	117.9	2.23
H4-O3-C1	107.1	104.1	94.5	112.9	2.89
O3-C5-O2-C1	0.4	-0.7	-11.5	11.7	3.80

1. J. C. Schoneboom, H. Lin, N. Reuter, W. Thiel, S. Cohen, F. Ogliaro and S. Shaik, *J. Am. Chem. Soc.*, 2002, **124**, 8142.

2. W. Humphrey, A. Dalke and K. Schulten, *J. Mol. Graphics*, 1996, **14**, 33.

3. K. Vanommeslaeghe, E. Hatcher, C. Acharya, S. Kundu, S. Zhong, J. Shim, E. Darian, O. Guvench, P. Lopes, I. Vorobyov and A. D. MacKerell, Jr., *J. Comput. Chem.*, 2010, **31**, 671.

Topology file of PFDA:

```
MASS   102 CX0   12.01100  C !
MASS   103 CX1   12.01100  C !
MASS   104 CX2   12.01100  C !
MASS   105 CX3   12.01100  C !
MASS   106 FX1   18.99840  F !
MASS   107 FX2   18.99840  F !
MASS   108 FX3   18.99840  F !
MASS   109 HX0    1.00800  H !
MASS   110 OX0   15.99900  O !
MASS   111 OX1   15.99900  O !

RESI PFDA          0.000   !   F31   F27 F24 F21 F18 F15 F12 F9  F7  O3-H4
GROUP                      !     \    |   |   |   |   |   |   |  /
ATOM   C1   CX0     0.70   ! F32-C29-C26-C23-C20-C17-C14-C11-C8--C5-C1
ATOM   O2   OX1    -0.53   !     /    |   |   |   |   |   |   |  \\
ATOM   O3   OX0    -0.58   !   F30   F28 F25 F22 F19 F16 F13 F10 F6  O2
ATOM   H4   HX0     0.43   !
ATOM   C5   CX1     0.36
ATOM   F6   FX1    -0.19
ATOM   F7   FX1    -0.19
ATOM  F10   FX2    -0.19
ATOM  C11   CX2     0.38
ATOM  F12   FX2    -0.19
ATOM  F13   FX2    -0.19
ATOM  C14   CX2     0.38
ATOM  F15   FX2    -0.19
ATOM  F16   FX2    -0.19
ATOM  C17   CX2     0.38
ATOM  F18   FX2    -0.19
ATOM  F19   FX2    -0.19
ATOM  C20   CX2     0.38
ATOM  F21   FX2    -0.19
ATOM  F22   FX2    -0.19
ATOM  C23   CX2     0.38
ATOM  F24   FX2    -0.19
ATOM  F25   FX2    -0.19
GROUP
ATOM  C26  CX2      0.36
ATOM  F27  FX2     -0.185
ATOM  F28  FX2     -0.185
ATOM  C29  CX3      0.445
ATOM  F30  FX3     -0.145
ATOM  F31  FX3     -0.145
ATOM  F32  FX3     -0.145

BOND   C1   O2    C1   O3    C1   C5    O3   H4
BOND   C5   F6    C5   F7    C5   C8    C8   F9
BOND   C8  F10    C8  C11   C11  F12   C11  F13
BOND  C11  C14   C14  F15   C14  F16   C14  C17
BOND  C17  F18   C17  F19   C17  C20   C20  F21
BOND  C20  F22   C20  C23   C23  F24   C23  F25
BOND  C23  C26   C26  F27   C26  F28   C26  C29
BOND  C29  F30   C29  F31   C29  F32

ANGLE   O2   C1   O3     O2   C1   C5     O3   C1   C5
ANGLE   C1   O3   H4     C1   C5   F6     C1   C5   F7
ANGLE   C1   C5   C8     F6   C5   F7     F6   C5   C8
ANGLE   F7   C5   C8     C5   C8   F9     C5   C8  F10
ANGLE   C5   C8  C11     F9   C8  F10     F9   C8  C11
ANGLE  F10   C8  C11     C8  C11  F12     C8  C11  F13
ANGLE   C8  C11  C14    F12  C11  F13    F12  C11  C14
ANGLE  F13  C11  C14    C11  C14  F15    C11  C14  F16
ANGLE  C11  C14  C17    F15  C14  F16    F15  C14  C17
ANGLE  F16  C14  C17    C14  C17  F18    C14  C17  F19
ANGLE  C14  C17  C20    F18  C17  F19    F18  C17  C20
ANGLE  F19  C17  C20    C17  C20  F21    C17  C20  F22
ANGLE  C17  C20  C23    F21  C20  F22    F21  C20  C23
ANGLE  F22  C20  C23    C20  C23  F24    C20  C23  F25
ANGLE  C20  C23  C26    F24  C23  F25    F24  C23  C26
ANGLE  F25  C23  C26    C23  C26  F27    C23  C26  F28
ANGLE  C23  C26  C29    F27  C26  F28    F27  C26  C29
ANGLE  F28  C26  C29    C26  C29  F30    C26  C29  F31
ANGLE  C26  C29  F32    F30  C29  F31    F30  C29  F32
ANGLE  F31  C29  F32

DIHED   O2   C1   O3   H4     C5   C1   O3   H4
DIHED   O2   C1   C5   F6     O2   C1   C5   F7
DIHED   O2   C1   C5   C8     O3   C1   C5   F6
DIHED   O3   C1   C5   F7     O3   C1   C5   C8
DIHED   C1   C5   C8   F9     C1   C5   C8  F10
DIHED   C1   C5   C8  C11     F6   C5   C8   F9
DIHED   F6   C5   C8  F10     F6   C5   C8  C11
DIHED   F7   C5   C8   F9     F7   C5   C8  F10
DIHED   F7   C5   C8  C11     C5   C8  C11  F12
DIHED   C5   C8  C11  F13     C5   C8  C11  C14
DIHED   F9   C8  C11  F12     F9   C8  C11  F13
DIHED   F9   C8  C11  C14    F10   C8  C11  F12
DIHED  F10   C8  C11  F13    F10   C8  C11  C14
DIHED   C8  C11  C14  F15     C8  C11  C14  F16
DIHED   C8  C11  C14  C17    F12  C11  C14  F15
DIHED  F12  C11  C14  F16    F12  C11  C14  C17
DIHED  F13  C11  C14  F15    F13  C11  C14  F16
DIHED  F13  C11  C14  C17    C11  C14  C17  F18
DIHED  C11  C14  C17  F19    C11  C14  C17  C20
DIHED  F15  C14  C17  F18    F15  C14  C17  F19
DIHED  F15  C14  C17  C20    F16  C14  C17  F18
DIHED  F16  C14  C17  F19    F16  C14  C17  C20
DIHED  C14  C17  C20  F21    C14  C17  C20  F22
DIHED  C14  C17  C20  C23    F18  C17  C20  F21
DIHED  F18  C17  C20  F22    F18  C17  C20  C23
DIHED  F19  C17  C20  F21    F19  C17  C20  F22
DIHED  F19  C17  C20  C23    C17  C20  C23  F24
DIHED  C17  C20  C23  F25    C17  C20  C23  C26
DIHED  F21  C20  C23  F24    F21  C20  C23  F25
DIHED  F21  C20  C23  C26    F22  C20  C23  F24
DIHED  F22  C20  C23  F25    F22  C20  C23  C26
DIHED  C20  C23  C26  F27    C20  C23  C26  F28
```

```
DIHED  C20  C23  C26  F27    C20  C23  C26  F28
DIHED  C20  C23  C26  C29    F24  C23  C26  F27
DIHED  F24  C23  C26  F28    F24  C23  C26  C29
DIHED  F25  C23  C26  F27    F25  C23  C26  F28
DIHED  F25  C23  C26  C29    C23  C26  C29  F30
DIHED  C23  C26  C29  F31    C23  C26  C29  F32
DIHED  F27  C26  C29  F30    F27  C26  C29  F31
DIHED  F27  C26  C29  F32    F28  C26  C29  F30
DIHED  F28  C26  C29  F31    F28  C26  C29  F32

IMPR O2 C5 O3 C1

DONOR H4 O3

ACCEPTOR O2 C1
ACCEPTOR O3 C1

PATCHING FIRS NONE LAST NONE

IC F7   C5   C8   F10   1.356  108.93 -163.03  107.60  1.357
IC F7   C5   C8   C11   1.356  108.93   76.53  114.19  1.558
IC C5   C8   C11  F12   1.556  114.19  -43.34  108.63  1.353
IC C5   C8   C11  F13   1.556  114.19   75.42  108.37  1.353
IC C5   C8   C11  C14   1.556  114.19 -163.68  113.41  1.561
IC F9   C8   C11  F12   1.353  108.96   78.12  108.63  1.353
IC F9   C8   C11  F13   1.353  108.96 -163.12  108.37  1.353
IC F9   C8   C11  C14   1.353  108.96  -42.21  113.41  1.561
IC F10  C8   C11  F12   1.357  108.46 -163.30  108.63  1.353
IC F10  C8   C11  F13   1.357  108.46  -44.54  108.37  1.353
IC F10  C8   C11  C14   1.357  108.46   76.37  113.41  1.561
IC C8   C11  C14  F15   1.558  113.41  -42.64  108.84  1.353
IC C8   C11  C14  F16   1.558  113.41   76.13  108.29  1.353
IC C8   C11  C14  C17   1.558  113.41 -163.04  113.37  1.561
IC F12  C11  C14  F15   1.353  108.20 -163.22  108.84  1.353
IC F12  C11  C14  F16   1.353  108.20  -44.45  108.29  1.353
IC F12  C11  C14  C17   1.353  108.20   76.38  113.37  1.561
IC F13  C11  C14  F15   1.353  108.79   78.03  108.84  1.353
IC F13  C11  C14  F16   1.353  108.79 -163.20  108.29  1.353
IC F13  C11  C14  C17   1.353  108.79  -42.37  113.37  1.561
IC C11  C14  C17  F18   1.561  113.37  -42.46  108.91  1.353
IC C11  C14  C17  F19   1.561  113.37   76.37  108.25  1.353
IC C11  C14  C17  C20   1.561  113.37 -162.88  113.26  1.561
IC F15  C14  C17  F18   1.353  108.16 -163.24  108.91  1.353
IC F15  C14  C17  F19   1.353  108.16  -44.42  108.25  1.353
IC F15  C14  C17  C20   1.353  108.16   76.33  113.26  1.561
IC F16  C14  C17  F18   1.353  108.80   78.09  108.91  1.353
IC F16  C14  C17  F19   1.353  108.80 -163.09  108.25  1.353
IC F16  C14  C17  C20   1.353  108.80  -42.33  113.26  1.561
IC C14  C17  C20  F21   1.561  113.26   76.39  108.29  1.353
IC C14  C17  C20  F22   1.561  113.26  -42.41  108.90  1.353
IC C14  C17  C20  C23   1.561  113.26 -162.78  113.32  1.560
IC F18  C17  C20  F21   1.353  108.18  -44.44  108.29  1.353
IC F18  C17  C20  F22   1.353  108.18 -163.25  108.90  1.353
IC F18  C17  C20  C23   1.353  108.18   76.39  113.32  1.560
IC F19  C17  C20  F21   1.353  108.82 -163.18  108.29  1.353
IC F19  C17  C20  F22   1.353  108.82   78.02  108.90  1.353
IC F19  C17  C20  C23   1.353  108.82  -42.34  113.32  1.560
IC C17  C20  C23  F24   1.561  113.32  -42.71  109.03  1.353
IC C17  C20  C23  F25   1.561  113.32   75.96  108.25  1.354
IC C17  C20  C23  C26   1.561  113.32 -163.23  113.58  1.556
IC F21  C20  C23  F24   1.353  108.83   77.82  109.03  1.353
IC F21  C20  C23  F25   1.353  108.83 -163.51  108.25  1.354
IC F21  C20  C23  C26   1.353  108.83  -42.71  113.58  1.556
IC F22  C20  C23  F24   1.353  108.12 -163.51  109.03  1.353
IC F22  C20  C23  F25   1.353  108.12  -44.84  108.25  1.354
IC F22  C20  C23  C26   1.353  108.12   75.96  113.58  1.556
IC C20  C23  C26  F27   1.560  113.58   75.21  108.61  1.351
IC C20  C23  C26  F28   1.560  113.58  -43.94  109.22  1.354
IC C20  C23  C26  C29   1.560  113.58 -164.53  114.18  1.553
IC F24  C23  C26  F27   1.353  108.04  -45.87  108.61  1.351
IC F24  C23  C26  F28   1.353  108.04 -165.02  109.22  1.354
IC F24  C23  C26  C29   1.353  108.04   74.39  114.18  1.553
IC F25  C23  C26  F27   1.354  108.69 -164.24  108.61  1.351
IC F25  C23  C26  F28   1.354  108.69   76.61  109.22  1.354
IC F25  C23  C26  C29   1.354  108.69  -43.97  114.18  1.553
IC C23  C26  C29  F30   1.556  114.18  -50.16  110.29  1.340
IC C23  C26  C29  F31   1.556  114.18   70.80  110.67  1.337
IC C23  C26  C29  F32   1.556  114.18 -169.63  108.91  1.338
IC F27  C26  C29  F30   1.351  107.76   70.57  110.29  1.340
IC F27  C26  C29  F31   1.351  107.76 -168.46  110.67  1.337
IC F27  C26  C29  F32   1.351  107.76  -48.90  108.91  1.338
IC F28  C26  C29  F30   1.354  107.67 -171.61  110.29  1.340
IC F28  C26  C29  F31   1.354  107.67  -50.65  110.67  1.337
IC F28  C26  C29  F32   1.354  107.67   68.91  108.91  1.338
END
```

Parameter file of PFDA:

```
BONDS
OX0  HX0     542.882    0.9769
CX0  OX0     258.151    1.3415
CX0  OX1     788.248    1.2013
CX0  CX1     177.447    1.5501
CX1  FX1     371.438    1.3527
CX1  CX2     212.207    1.5555
CX2  FX2     383.700    1.3533
CX2  CX2     205.2198   1.5595
CX2  CX3     207.354    1.5530
CX3  FX3     401.534    1.3383

ANGLES
OX1  CX0  OX0      46.377    126.20  194.78  2.268
OX1  CX0  CX1      66.728    123.53   19.06  2.430
OX0  CX0  CX1      53.050    110.26
CX0  OX0  HX0      54.000    107.12
CX0  CX1  FX1      51.369    108.70  46.70   2.362
CX0  CX1  CX2      66.091    112.32
FX1  CX1  FX1      69.357    109.26  10.55   2.206
FX1  CX1  CX2      44.474    108.91  37.81   2.369
CX1  CX2  FX2      43.394    108.05  36.89   2.358
CX1  CX2  CX2      84.314    114.19  16.13   2.614
FX2  CX2  FX2       65.87    109.16  10.00   2.207
FX2  CX2  CX2      43.819    108.57  37.25   2.368
CX2  CX2  CX2      89.376    113.39  17.09   2.608
CX2  CX2  CX3      85.877    114.18  11.85   2.610
FX2  CX2  CX3      56.103    107.72  36.53   2.349
CX2  CX3  FX3      63.800    109.96  41.54   2.371
FX3  CX3  FX3      80.626    108.97  12.26   2.179


DIHEDRALS
OX1  CX0  OX0  HX0      2.05     2    180.00
CX1  CX0  OX0  HX0      2.05     2    180.00
OX1  CX0  CX1  FX1      0.00     6    180.00
OX1  CX0  CX1  CX2      0.00     6    180.00
OX0  CX0  CX1  FX1      0.00     6    180.00
OX0  CX0  CX1  CX2      0.00     6    180.00
CX0  CX1  CX2  FX2      0.35     3      0.00
CX0  CX1  CX2  CX2      0.35     3      0.00
CX1  CX2  CX2  FX2      0.35     3      0.00
FX1  CX1  CX2  FX2      0.35     3      0.00
FX1  CX1  CX2  CX2      0.35     3      0.00
CX1  CX2  CX2  CX2      0.35     3      0.00
FX2  CX2  CX2  FX2      0.35     3      0.00
FX2  CX2  CX2  CX2      0.35     3      0.00
FX2  CX2  CX2  CX3      0.35     3      0.00
CX2  CX2  CX3  FX3      0.35     3      0.00
FX2  CX2  CX3  FX3      0.35     3      0.00
CX2  CX2  CX2  CX3      0.25     1      0.00
CX2  CX2  CX2  CX2      0.25     1      0.00

improper
OX1  CX1  OX0  CX0  100.0000     0      0.000


NONBONDED
CX0       0.0     -0.0700     2.0000    !
OX1       0.0     -0.1200     1.7000    0.0
OX0       0.0     -0.1521     1.7700    !
HX0       0.0     -0.0460     0.2245    !
CX1       0.0     -0.0420     2.0500    !
FX1       0.0     -0.1050     1.6300    !
CX2       0.0     -0.0420     2.0500    !
FX2       0.0     -0.1050     1.6300    !
CX3       0.0     -0.0200     2.3000    !
FX3       0.0     -0.0970     1.6000    !
```

4. QM/MM results:

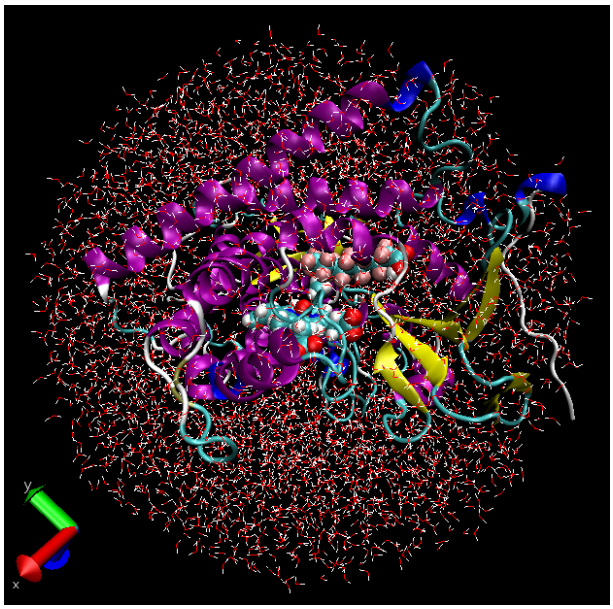
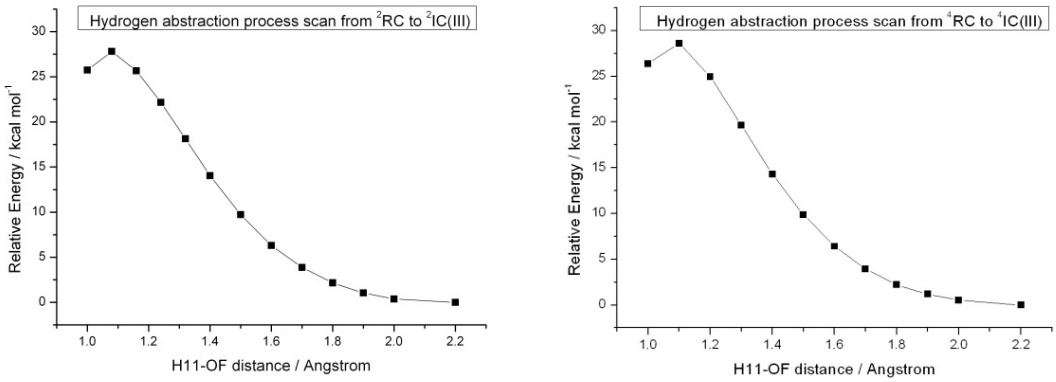
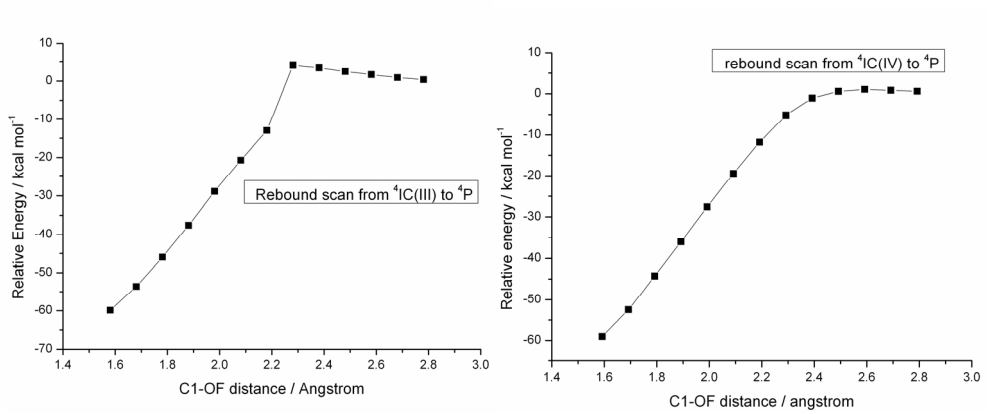


Figure S1. P450BM3 with solvent shell from partial solvation setup. PFDA, methane and Cpd I are shown in VDW model. Waters are shown in lines.



(a) (b)

Figure S2. Energy scans for hydrogen abstraction process starting (a) from ^{2}RC to ^{2}IC(III) and (b) from ^{4}RC to ^{4}IC(III). H11 is hydrogen atoms of methane abstracted to OF, the ferryl-oxo oxygen atom, of Cpd I.



(a) (b)

Figure S3. Energy scans for rebound process starting from radical intermediates (a) ^{4}IC(III) and (b) ^{4}IC(IV) to hydroxylated products. C1 is carbon atoms of methane and OF is ferryl-oxo oxygen atom of Cpd I.

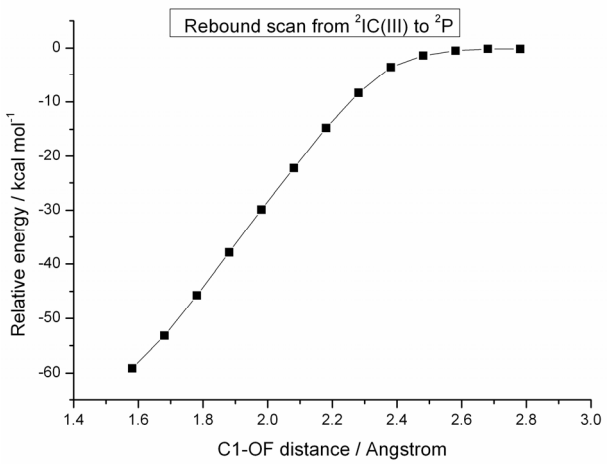


Figure S4. Energy scans for rebound process starting from ^{2}IC(III) to hydroxylated products. C1 is carbon atoms of methane and OF is ferryl-oxo oxygen atom of Cpd I.

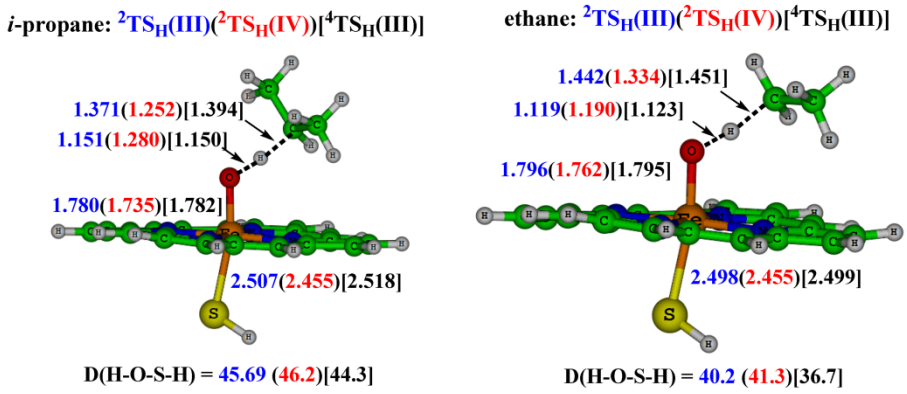


Figure S5. Geometry structures of the QM/MM optimized hydrogen abstraction transition states of *i*-propane and ethane hydroxylation by Cpd I at B3LYP/B1 level.

Table S2. QM/MM computed relative Energy (in kcal mol^{-1}) of the species in methane hydroxylation by Cpd I from SnapX1 and SnapX2 at virous computational levels.

	B1	B1+ZPE	B2	B2+ZPE	B3	B3+ZPE
	SnapX1					
^{2}RC	0.0	0.0	0.0	0.0	0.0	0.0
^{4}RC	-0.1	0.0	-0.1	0.0	0.1	0.1
$^{2}TS_{H}$(III)	27.3	22.9	23.5	19.1	26.1	21.7
$^{2}TS_{H}$(IV)	28.5	25.1	21.7	18.2	22.2	18.8
$^{4}TS_{H}$(III)	28.0	23.6	24.4	20.0	27.0	22.7
^{2}IC(III)	24.9	22.6	17.7	15.4	20.8	18.5
^{2}IC(IV)	25.8	23.9	14.9	13.0	15.5	13.6
^{4}IC(III)	25.4	22.3	18.1	15.1	21.2	18.1
^{4}IC(IV)	26.2	24.2	15.1	13.1	15.8	13.7
^{4}TSreb(III)	29.4	26.4	22.4	19.4	25.9	22.9
^{2}P	-37.2	-34.6	-48.0	-45.4	-44.4	-41.8
^{4}P	-38.1	-36.6	-50.2	-48.8	-46.2	-44.7
	SnapX2					
^{2}RC	0.0	0.0	0.0	0.0		
^{4}RC	-0.1	0.2	0.0	0.4		
$^{2}TS_{H}$(III)	27.9	24.7	23.6	20.5		
$^{2}TS_{H}$(IV)	28.5	25.3	21.3	19.5		
$^{4}TS_{H}$(III)	28.7	25.1	24.7	21.2		
^{2}IC(III)	25.9	24.2	18.4	16.9		
^{2}IC(IV)	25.4	23.7	14.0	12.3		
^{4}IC(III)	26.3	24.4	18.8	17.0		
^{4}IC(IV)	26.9	25.0	15.2	13.3		
^{4}TSreb(III)	32.4	29.6	25.0	22.2		
^{2}P	-34.7	-32.5	-46.0	-43.3		
^{4}P	-35.0	-33.1	-47.8	-45.7		

Table S3. QM/MM computed relative Energy (in kcal mol^{-1}) of the species in ethane hydroxylation by Cpd I at virous computational levels.

	B1	B1+ZPE	B2	B2+ZPE	B3	B3+ZPE
^{2}RC	0.0	0.0	0.0	0.0	0.0	0.0
^{4}RC	-0.1	0.0	0.0	0.1	0.1	0.3
$^{2}TS_{H}$(III)	22.6	18.6	19.7	15.7	22.5	18.5
$^{2}TS_{H}$(IV)	23.8	19.8	17.9	13.9	18.5	14.5
$^{4}TS_{H}$(III)	23.5	19.6	20.7	16.8	23.5	19.6
^{2}IC(III)	18.1	16.1	10.8	8.8	14.0	12.0
^{2}IC(IV)	18.6	16.6	7.8	5.8	8.4	6.4
^{4}IC(III)	17.9	16.0	10.7	8.8	13.7	11.9
^{4}IC(IV)	19.1	17.9	8.1	6.9	8.4	7.2
^{4}TSreb(III)	21.8	18.8	14.8	11.8	18.3	15.2
^{2}P	-42.3	-40.2	-53.4	-51.2	-49.7	-47.5
^{4}P	-45.0	-43.8	-57.3	-56.1	-53.3	-52.1

Table S4. QM/MM computed relative Energy (in kcal mol^{-1}) of the species in *i*-propane hydroxylation by Cpd I at virous computational levels.

	B1	B1+ZPE	B2	B2+ZPE	B3	B3+ZPE
^{2}RC	0.0	0.0	0.0	0.0	0.0	0.0
^{4}RC	-0.2	0.1	-0.1	0.1	0.1	0.3
$^{2}TS_{H}$(III)	17.9	13.3	16.3	11.7	18.6	9.3
$^{2}TS_{H}$(IV)	18.7	14.7	14.5	10.5	14.8	10.8
$^{4}TS_{H}$(III)	19.0	15.2	17.7	13.8	20.3	16.4
^{2}IC(III)	13.8	12.0	7.7	5.9	10.6	8.9
^{2}IC(IV)	13.5	11.1	4.1	1.7	4.6	2.3
^{4}IC(III)	14.3	11.6	8.1	5.5	11.1	8.5
^{4}IC(IV)	14.2	11.9	4.5	2.3	5.1	2.8
^{4}TSreb(III)	18.7	16.1	12.8	10.2	16.4	13.8
^{2}P	-47.0	-45.3	-55.6	-53.9	-51.4	-49.7
^{4}P	-49.4	-47.8	-60.2	-58.7	-56.2	-54.7

Table S5. QM/MM computed mulliken group spin densities (ρ) and NBO charges (Q) of the species in methane hydroxylation by Cpd I at B3LYP/B2//B1 level.

	ρ						
	Fe	O	Por	SH	substrate		
					H	C	sub-H
^{2}RC	1.33	0.86	-0.89	-0.31			
^{4}RC	1.12	0.92	0.70	0.25			
^{2}TS$_{H}$(III)	1.03	0.36	-0.84	-0.22	-0.04	0.78	0.71
^{2}TS$_{H}$(IV)	1.95	-0.03	-0.14	-0.17	0.02	-0.69	-0.63
^{4}TS$_{H}$(III)	0.79	0.45	0.90	0.19	-0.05	0.78	0.71
^{2}IC(III)	1.09	0.10	-0.92	-0.21	0.00	1.08	0.96
^{2}IC(IV)	1.99	0.18	-0.09	-0.13	-0.01	-1.06	-0.94
^{4}IC(III)	0.79	0.18	0.90	0.17	-0.01	1.09	0.96
^{4}IC(IV)	1.97	0.21	-0.05	-0.10	0.02	1.08	0.96
^{4}TSreb(III)	1.03	-0.11	0.94	0.26	0.03	0.95	0.84
^{2}P	0.97	-0.01	0.04	-0.01	0.00	0.00	0.01
^{4}P	2.97	-0.02	-0.26	0.30	0.00	0.00	0.01
	Q						
	Fe	O	Por	SH	substrate		
					H	C	sub-H
^{2}RC	0.95	-0.47	-0.02	-0.45			
^{4}RC	0.93	-0.46	-0.02	-0.45			
^{2}TS$_{H}$(III)	0.99	-0.77	-0.10	-0.45	0.38	-0.60	-0.04
^{2}TS$_{H}$(IV)	1.11	-0.69	-0.45	-0.34	0.36	-0.57	0.01
^{4}TS$_{H}$(III)	0.98	-0.76	-0.09	-0.46	0.38	-0.60	-0.05
^{2}IC(III)	0.99	-0.87	-0.10	-0.46	0.44	-0.50	0.00
^{2}IC(IV)	1.14	-0.82	-0.46	-0.34	0.46	-0.50	0.01
^{4}IC(III)	0.98	-0.87	-0.08	-0.47	0.44	-0.50	0.00
^{4}IC(IV)	1.14	-0.82	-0.46	-0.34	0.46	-0.50	0.01
^{4}TSreb(III)	1.03	-0.86	-0.19	-0.47	0.45	-0.45	0.04
^{2}P	0.98	-0.73	-0.77	-0.34	0.51	-0.20	0.35
^{4}P	1.33	-0.77	-0.81	-0.57	0.49	-0.20	0.32

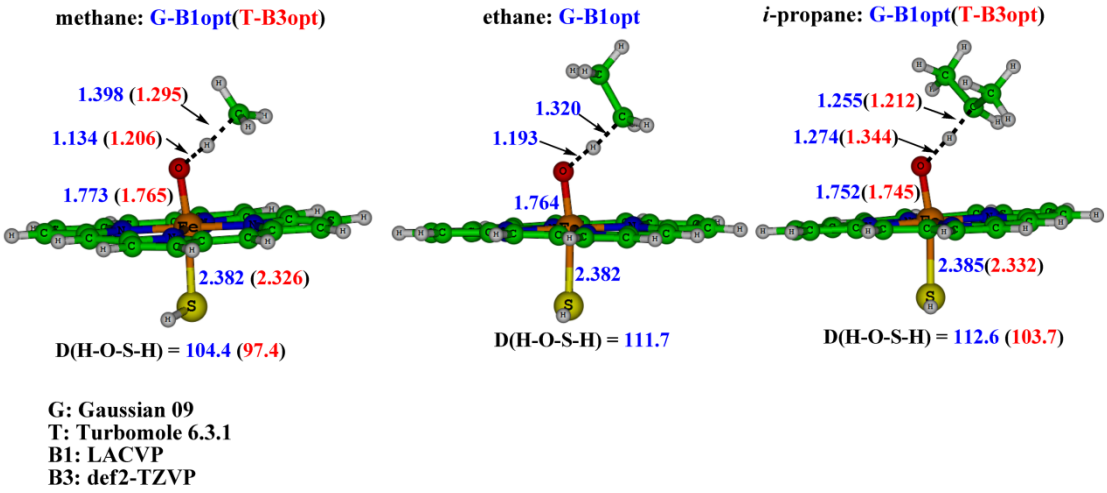
Table S6. QM/MM computed mulliken group spin densities (ρ) and NBO charges (Q) of the species in ethane hydroxylation by Cpd I at B3LYP/B2//B1 level.

	ρ						
	Fe	O	Por	SH	substrate		
					H	C	sub-H
^{2}RC	1.34	0.87	-0.91	-0.30			
^{4}RC	1.10	0.92	0.73	0.24			
^{2}TS$_{H}$(III)	1.05	0.40	-0.77	-0.21	-0.04	0.64	0.58
^{2}TS$_{H}$(IV)	1.85	-0.08	-0.09	-0.14	0.01	-0.53	-0.54
^{4}TS$_{H}$(III)	0.80	0.49	0.88	0.20	-0.05	0.68	0.67
^{2}IC(III)	1.03	0.08	-0.90	-0.19	0.01	1.06	0.97
^{2}IC(IV)	1.97	0.19	-0.07	-0.12	-0.01	-1.03	-0.96
^{4}IC(III)	0.75	0.16	0.92	0.18	-0.01	1.08	0.99
^{4}IC(IV)	1.92	0.19	-0.01	-0.11	0.03	1.05	0.98
^{4}TSreb(III)	1.00	-0.09	0.98	0.24	0.03	0.92	0.83
^{2}P	0.95	-0.01	0.11	-0.05	0.00	0.00	0.00
^{4}P	2.96	-0.02	-0.24	0.30	0.00	0.00	0.00
	Q						
	Fe	O	Por	SH	substrate		
					H	C	sub-H
^{2}RC	0.94	-0.47	-0.02	-0.46			
^{4}RC	0.93	-0.46	-0.02	-0.46			
^{2}TS$_{H}$(III)	0.98	-0.73	-0.13	-0.45	0.36	-0.40	-0.03
^{2}TS$_{H}$(IV)	1.10	-0.64	-0.45	-0.36	0.34	-0.39	0.02
^{4}TS$_{H}$(III)	0.98	-0.73	-0.09	-0.47	0.36	-0.41	-0.05
^{2}IC(III)	0.99	-0.88	-0.09	-0.47	0.44	-0.29	0.00
^{2}IC(IV)	1.14	-0.82	-0.45	-0.35	0.46	-0.30	0.01
^{4}IC(III)	0.97	-0.88	-0.08	-0.46	0.44	-0.29	0.00
^{4}IC(IV)	1.14	-0.82	-0.45	-0.35	0.47	-0.29	0.01
^{4}TSreb(III)	1.02	-0.87	-0.18	-0.49	0.45	-0.22	0.07
^{2}P	1.02	-0.77	-0.77	-0.34	0.51	-0.01	0.35
^{4}P	1.34	-0.79	-0.80	-0.57	0.50	-0.02	0.32

Table S7. QM/MM computed mulliken group spin densities (ρ) and NBO charges (Q) of the species in *i*-propane hydroxylation by Cpd I at B3LYP/B2//B1 level.

	ρ						
	Fe	O	Por	SH	substrate		
					H	C	sub-H
^{2}RC	1.36	0.89	-0.97	-0.27			
^{4}RC	1.11	0.95	0.74	0.21			
^{2}TS$_{H}$(III)	1.02	0.42	-0.71	-0.22	-0.02	0.48	0.49
^{2}TS$_{H}$(IV)	1.72	-0.12	-0.08	-0.12	0.00	-0.38	-0.40
^{4}TS$_{H}$(III)	0.70	0.54	0.99	0.19	-0.02	0.59	0.60
^{2}IC(III)	1.03	0.10	-0.86	-0.19	0.00	0.95	0.93
^{2}IC(IV)	1.86	0.22	-0.08	-0.11	0.01	-0.91	-0.90
^{4}IC(III)	0.68	0.18	1.03	0.16	0.00	0.98	0.95
^{4}IC(IV)	1.82	0.23	0.08	-0.08	0.02	0.95	0.93
^{4}TSreb(III)	0.91	-0.07	1.07	0.23	0.03	0.84	0.82
^{2}P	1.00	-0.01	0.07	-0.08	0.01	0.00	0.01
^{4}P	2.99	-0.01	-0.26	0.29	-0.01	-0.01	0.00
	Q						
	Fe	O	Por	SH	substrate		
					H	C	sub-H
^{2}RC	0.94	-0.45	-0.01	-0.48			
^{4}RC	0.93	-0.44	0.00	-0.49			
^{2}TS$_{H}$(III)	0.98	-0.69	-0.15	-0.47	0.34	-0.22	-0.01
^{2}TS$_{H}$(IV)	1.09	-0.57	-0.41	-0.39	0.31	-0.25	-0.02
^{4}TS$_{H}$(III)	0.98	-0.70	-0.09	-0.49	0.36	-0.24	-0.06
^{2}IC(III)	1.00	-0.86	-0.12	-0.50	0.44	-0.11	0.03
^{2}IC(IV)	1.13	-0.79	-0.47	-0.38	0.46	-0.12	0.04
^{4}IC(III)	0.99	-0.85	-0.09	-0.50	0.44	-0.12	0.01
^{4}IC(IV)	1.14	-0.79	-0.47	-0.37	0.47	-0.12	0.03
^{4}TSreb(III)	1.03	-0.87	-0.22	-0.50	0.45	-0.02	0.12
^{2}P	1.04	-0.75	-0.73	-0.40	0.50	0.12	0.35
^{4}P	1.35	-0.78	-0.79	-0.58	0.48	0.12	0.32

5. QM results:



G: Gaussian 09
T: Turbomole 6.3.1
B1: LACVP
B3: def2-TZVP

Figure S6. Geometry structures of the QM optimized $^{2}TS_{H}$(IV) of methane, *i*-propane and ethane hydroxylation by Cpd I at various levels.

Abbreviations:

G: Gaussian09; J: Jaguar7.8; T: Turbomole6.3.1;

B1: LACVP; B2: LACV3P++**; B3: def2-TZVP; B4: LACV3P+*; B5: Wachters full electron (Fe)/6-311++G**(rest)

B6: aug-cc-pVTZ

Ref 4: S. Shaik, D. Kumar and S. P. de Visser, *J. Am. Chem. Soc.*, 2008, **130**, 10128.

Table S8. Barriers (in kcal mol^{-1}) relative to separated reactant ^{2}Cpd I + Alk-H using G-B1 optimized geometry structure. Data are given as $\Delta E^{\ddagger}$+ZPE‡ and ZPE‡ are from G-B1.

		G-B1 optimization							
		G-B1	G-B2//G-B1	J-B2//G-B1	G-B4//G-B1	J-B4//G-B1	T-B3//G-B1	G-B5//G-B1	G-B6//G-B1
methane	$^2TS_H(III)^a$	22.2	19.1	19.0	22.0	22.3[c]	22.3		
	$^2TS_H(IV)^b$	21.4	15.2	15.6	18.0	19.0	16.5	16.1	19.2
i-propane	$^2TS_H(IV)^a$	14.1	10.9	11.5	12.7	13.9[c]	12.4		
	$^2TS_H(IV)^b$	13.4	9.8	10.4	11.5	12.5	11.2		

[a]Geometry structure of the transition states are from ref. 4; [b]This work. [c]These are the data published in Table 1 of ref. 4.

Table S9. Barriers (in kcal mol^{-1}) relative to separated reactant ^{2}Cpd I + Alk-H using T-B3 optimized geometry structure. Data are given as $\Delta E^{\ddagger}$+ZPE‡ and ZPE‡ are from T-B3.

	T-B3	G-B2//T-B3	J-B2//T-B3	G-B4//T-B3	J-B4//T-B3	T-B6//T-B3
Methane: $^2TS_H(IV)^a$	18.1	17.1	17.4	19.2	19.9	17.4
i-propane: $^2TS_H(IV)^a$	12.1	10.9	11.6	12.2	12.9	11.6

[a]This work.

Table S10. QM computed mulliken group spin densities (ρ) and NBO charges (Q) of the ^2TS_H(IV) in methane, ethane and *i*-propane hydroxylation by Cpd I at B3LYP/B1 and B3LYP/B3 level.

	Alkane	Level	ρ						
			Fe	O	Por	SH	substrate		
							H	C	sub-H
^2TS_H(IV)	Methane	G-B1[a]	1.83	-0.02	-0.17	-0.08	0.04	-0.68	-0.60
		T-B3[b]	1.85	-0.19	-0.19	-0.01	0.04	-0.52	-0.50
^2TS_H(IV)	Ethane	G-B1[a]	1.78	-0.07	-0.16	-0.06	0.03	-0.54	-0.52
^2TS_H(IV)	*i*-propane	G-B1[a]	1.75	-0.11	-0.18	-0.07	0.03	-0.41	-0.41
		T-B3[b]	1.80	-0.26	-0.22	0.00	0.02	-0.31	-0.34
	Alkane	Level	Q						
			Fe	O	Por	SH	substrate		
							H	C	sub-H
^2TS_H(IV)	Methane	G-B1[a,c]	1.00	-0.63	-0.50	-0.24	0.39	-0.72	-0.02
		T-B3[b,d]	1.02	-0.61	-0.52	-0.18	0.31	-0.64	-0.03
^2TS_H(IV)	Ethane	G-B1[a,c]	0.98	-0.59	-0.50	-0.25	0.37	-0.52	-0.01
^2TS_H(IV)	*i*-propane	G-B1[a,c]	0.85	-0.51	-0.39	-0.20	0.35	-0.36	-0.10
		T-B3[b,d]	1.01	-0.56	-0.50	-0.20	0.29	-0.27	-0.05

[a]G-B1: B3LYP/LACVP optimization by Gaussian 09. [b]T-B3: B3LYP/def2-TZVP optimization by Turbomole 6.3.1. [c]Charges are calculated by NBO 5.0 embedded in Jaguar 7.8. [d]Charges are calculated by NBO embedded in Turbomole 6.3.1.

Cartesian Coordinates of the QM Region of the Optimized Species from QM/MM calculation

Methane reaction:

^{2}RC

S	0.507907	-1.773096	3.840765
O	0.155013	-0.059389	0.008469
Fe	0.307372	-0.858906	1.449608
N	0.209296	-2.701282	0.572645
N	-1.700788	-0.890944	1.754180
N	0.456629	0.849110	2.540889
N	2.328503	-0.941510	1.296321
C	1.254151	-3.481658	0.089707
C	0.738524	-4.662784	-0.599799
C	-0.636304	-4.573791	-0.552798
C	-0.952091	-3.358967	0.189835
C	-2.602693	-1.792126	1.225214
C	-3.972666	-1.422446	1.578276
C	-3.891781	-0.289593	2.372034
C	-2.453451	0.026187	2.463327
C	-0.557053	1.474048	3.234368
C	-0.055694	2.650534	3.946310
C	1.286680	2.761001	3.637150
C	1.587168	1.618774	2.753498
C	3.190769	0.108036	1.561781
C	4.542430	-0.220071	1.125071
C	4.502913	-1.511419	0.644162
C	3.109392	-1.941816	0.722633
C	2.598986	-3.126743	0.197996
H	3.320153	-3.818083	-0.224628
C	-2.237319	-2.923867	0.494670
H	-3.044499	-3.562101	0.149889
C	-1.889902	1.077761	3.185362
H	-2.580673	1.684942	3.757496
C	2.833551	1.274829	2.236112
H	3.648994	1.964041	2.432405
C	-1.212829	-0.580302	-2.902047
H	-0.754539	-0.283401	-1.956275
H	-0.563334	-0.285889	-3.732305
H	-1.350036	-1.666796	-2.913212
H	-2.183131	-0.087890	-3.022012
h	0.634628	-3.146010	3.782477
h	1.330639	-5.437857	-1.086346
h	-1.386116	-5.230006	-0.994647
h	-4.834118	-1.978584	1.208578
h	-4.659537	0.329950	2.835481
h	-0.713566	3.277228	4.548410
h	2.034994	3.509789	3.896785
h	5.383087	0.473544	1.141194
h	5.325935	-2.104415	0.245341

^{2}TS$_{H}$(III)

S	0.516583	-1.759926	3.779311
O	0.234851	0.076076	-0.072590
Fe	0.294720	-0.890081	1.441014
N	0.173744	-2.696398	0.497628
N	-1.718333	-0.904294	1.693187
N	0.455665	0.848305	2.501738
N	2.318654	-0.955972	1.274977
C	1.222378	-3.475785	0.020744
C	0.712844	-4.669536	-0.652761
C	-0.663024	-4.598214	-0.589755
C	-0.985007	-3.381570	0.146609
C	-2.629497	-1.816724	1.192988
C	-3.992718	-1.443385	1.560818
C	-3.901085	-0.299782	2.340213
C	-2.461213	0.018714	2.406442
C	-0.562210	1.475108	3.183395
C	-0.063916	2.647958	3.909588
C	1.282251	2.750616	3.619338
C	1.585871	1.606121	2.735025
C	3.186796	0.083619	1.552892
C	4.537945	-0.248623	1.113256
C	4.489127	-1.532162	0.614452
C	3.090186	-1.952162	0.685046
C	2.569314	-3.123607	0.139980
H	3.288740	-3.816167	-0.284564
C	-2.269726	-2.959658	0.476325
H	-3.077727	-3.613910	0.163067
C	-1.893088	1.074868	3.124734
H	-2.584794	1.678356	3.700633
C	2.835764	1.249375	2.233383
H	3.656509	1.928898	2.442649

C	-1.081197	-0.596867	-2.187152
H	-0.342520	-0.296344	-0.910026
H	-0.361303	-0.237305	-2.919094
H	-1.231249	-1.672398	-2.137560
H	-1.963105	0.025402	-2.056730
h	0.635121	-3.133694	3.724023
h	1.310025	-5.446234	-1.130446
h	-1.409204	-5.268895	-1.015746
h	-4.859419	-2.004922	1.212147
h	-4.663136	0.318323	2.814862
h	-0.725423	3.271099	4.511394
h	2.034275	3.491502	3.890658
h	5.385320	0.436430	1.140152
h	5.310111	-2.127943	0.215583

^{2}IC(III)

S	0.518336	-1.763407	3.805134
O	0.225003	0.062016	-0.075667
Fe	0.318977	-0.881532	1.483605
N	0.193415	-2.687096	0.517312
N	-1.700918	-0.896479	1.720472
N	0.473269	0.856473	2.528034
N	2.335737	-0.943860	1.301412
C	1.240357	-3.467044	0.041931
C	0.731122	-4.656539	-0.639908
C	-0.645213	-4.580052	-0.584888
C	-0.966137	-3.364207	0.153589
C	-2.611977	-1.801882	1.206980
C	-3.976609	-1.427192	1.569251
C	-3.885834	-0.287719	2.355327
C	-2.445196	0.025758	2.430876
C	-0.545471	1.483009	3.208729
C	-0.049121	2.660730	3.929183
C	1.295654	2.767201	3.634545
C	1.600585	1.620330	2.753377
C	3.200901	0.099106	1.566950
C	4.550978	-0.229934	1.121510
C	4.504527	-1.516731	0.630721
C	3.107061	-1.941358	0.710796
C	2.587933	-3.113981	0.166672
H	3.308608	-3.805415	-0.257730
C	-2.251181	-2.938378	0.479551
H	-3.059996	-3.586155	0.154500
C	-1.876421	1.082108	3.149998
H	-2.569119	1.688383	3.721661
C	2.848507	1.267471	2.244502
H	3.667665	1.951653	2.444659
C	-1.224383	-0.635555	-2.641540
H	-0.317581	-0.395374	-0.762601
H	-0.368107	-0.259124	-3.188126
H	-1.367276	-1.702952	-2.518480
H	-1.996109	0.058270	-2.331967
h	0.633924	-3.137249	3.745613
h	1.327009	-5.433676	-1.118493
h	-1.392209	-5.248477	-1.012990
h	-4.842630	-1.985857	1.214333
h	-4.648713	0.330080	2.829044
h	-0.711864	3.283880	4.529616
h	2.045903	3.512008	3.899981
h	5.394879	0.459669	1.140104
h	5.325088	-2.111895	0.230065

^{2}TS$_{H}$(IV)

S	0.495545	-1.759008	3.736324
O	0.227177	0.056350	-0.035747
Fe	0.308731	-0.903733	1.448103
N	0.194590	-2.691948	0.518906
N	-1.709045	-0.900597	1.700782
N	0.453899	0.828852	2.514940
N	2.327166	-0.962668	1.265419
C	1.252821	-3.480319	0.047165
C	0.732595	-4.664363	-0.623416
C	-0.644679	-4.584119	-0.567613
C	-0.972222	-3.370719	0.164688
C	-2.613645	-1.816806	1.190510
C	-3.976892	-1.439495	1.552347
C	-3.891391	-0.299676	2.337439
C	-2.454912	0.024871	2.417969
C	-0.571315	1.461969	3.189677
C	-0.065110	2.631421	3.906741
C	1.284073	2.727165	3.619176
C	1.591919	1.582276	2.742457
C	3.186116	0.086543	1.550512
C	4.535997	-0.243635	1.108771
C	4.494557	-1.529975	0.615367
C	3.100947	-1.960372	0.684618
C	2.596353	-3.144525	0.159237
H	3.315336	-3.841015	-0.256149

C	-2.260966	-2.956819	0.475582
H	-3.064976	-3.610870	0.156212
C	-1.903245	1.080406	3.134835
H	-2.593825	1.689959	3.703445
C	2.844052	1.241555	2.241995
H	3.662637	1.919988	2.457266
C	-1.052009	-0.578220	-2.127836
H	-0.367626	-0.271330	-0.935811
H	-0.340633	-0.255127	-2.885760
H	-1.211179	-1.650207	-2.038875
H	-1.936677	0.047557	-2.030633
h	0.625641	-3.131978	3.687581
h	1.324894	-5.442761	-1.104400
h	-1.389913	-5.252161	-0.999367
h	-4.841908	-1.998915	1.196167
h	-4.657634	0.312519	2.812997
h	-0.724067	3.263365	4.502131
h	2.034402	3.470298	3.889041
h	5.379656	0.446143	1.131427
h	5.318665	-2.123412	0.219455

^{2}IC(IV)

S	0.492988	-1.771864	3.751317
O	0.228404	0.046704	-0.043778
Fe	0.325531	-0.888045	1.488763
N	0.207548	-2.673771	0.534311
N	-1.699473	-0.881196	1.722623
N	0.463913	0.833556	2.547816
N	2.339150	-0.954178	1.299567
C	1.264408	-3.466748	0.068288
C	0.742767	-4.645603	-0.609237
C	-0.634825	-4.556707	-0.564426
C	-0.960439	-3.342405	0.167280
C	-2.602347	-1.792246	1.199586
C	-3.966869	-1.416793	1.559892
C	-3.883713	-0.281975	2.352415
C	-2.447409	0.040732	2.440962
C	-0.562722	1.468253	3.221472
C	-0.056541	2.641146	3.930965
C	1.291662	2.740308	3.636427
C	1.600234	1.593388	2.763819
C	3.195057	0.098764	1.572783
C	4.543548	-0.229648	1.125227
C	4.503600	-1.518913	0.639062
C	3.111619	-1.953129	0.717167
C	2.608491	-3.136706	0.189711
H	3.328010	-3.835152	-0.221261
C	-2.249403	-2.924511	0.473021
H	-3.053396	-3.573130	0.142971
C	-1.895978	1.091404	3.164499
H	-2.587170	1.702359	3.730495
C	2.851667	1.256991	2.258547
H	3.668572	1.939537	2.466801
C	-1.212535	-0.624280	-2.588597
H	-0.308556	-0.352913	-0.775829
H	-0.373671	-0.271238	-3.177541
H	-1.356660	-1.686907	-2.428381
H	-1.995396	0.075620	-2.321825
h	0.627605	-3.144200	3.697306
h	1.332029	-5.426346	-1.090149
h	-1.381068	-5.222830	-0.997403
h	-4.830484	-1.976125	1.200191
h	-4.651769	0.328715	2.826982
h	-0.715140	3.274585	4.525161
h	2.039417	3.489100	3.897655
h	5.384416	0.463745	1.139835
h	5.325961	-2.111757	0.238656

^{2}P

S	0.461851	-1.774505	3.763188
O	0.022690	0.280517	-0.124499
Fe	0.278562	-0.918397	1.604256
N	0.156792	-2.655152	0.532374
N	-1.750341	-0.839051	1.760951
N	0.386558	0.893339	2.535250
N	2.261140	-0.920252	1.267962
C	1.200790	-3.448793	0.056704
C	0.674616	-4.633571	-0.619836
C	-0.699518	-4.543292	-0.558872
C	-1.011771	-3.323187	0.183120
C	-2.649398	-1.758998	1.238193
C	-4.017017	-1.389446	1.593138
C	-3.942421	-0.251826	2.387073
C	-2.508612	0.075243	2.480843
C	-0.625571	1.519344	3.249407
C	-0.103414	2.671037	3.982418
C	1.245060	2.759643	3.686685
C	1.536752	1.628150	2.785021

C	3.125525	0.120548	1.573700
C	4.480333	-0.211232	1.141824
C	4.440847	-1.496000	0.641211
C	3.045078	-1.922207	0.696086
C	2.545598	-3.109369	0.169877
H	3.268001	-3.806380	-0.240373
C	-2.294056	-2.893311	0.506988
H	-3.104078	-3.538570	0.183070
C	-1.957867	1.134790	3.201111
H	-2.649607	1.739368	3.774437
C	2.785246	1.273211	2.278502
H	3.611866	1.938278	2.507587
C	-0.705350	-0.094055	-1.340213
H	-0.325157	1.098667	0.288299
H	-0.455049	0.603836	-2.144245
H	-0.360547	-1.095890	-1.587161
H	-1.783200	-0.108441	-1.157261
h	0.613380	-3.144283	3.691809
h	1.266728	-5.414659	-1.096671
h	-1.450432	-5.207092	-0.987316
h	-4.878697	-1.951241	1.232639
h	-4.712485	0.353379	2.865399
h	-0.748787	3.292604	4.603075
h	2.006169	3.487332	3.968194
h	5.327838	0.473559	1.171186
h	5.266292	-2.085080	0.241594

^{4}RC

S	0.512911	-1.768451	3.832445
O	0.156096	-0.064780	0.016219
Fe	0.310936	-0.864021	1.458497
N	0.209666	-2.700639	0.571716
N	-1.701116	-0.890187	1.752773
N	0.456675	0.849290	2.541307
N	2.328091	-0.943475	1.299341
C	1.254416	-3.481911	0.090610
C	0.738840	-4.662407	-0.599967
C	-0.635863	-4.573215	-0.553093
C	-0.952129	-3.358302	0.189217
C	-2.602958	-1.791449	1.223751
C	-3.972925	-1.421894	1.577151
C	-3.892232	-0.289238	2.371205
C	-2.453678	0.026433	2.462599
C	-0.557065	1.473446	3.235646
C	-0.055859	2.650234	3.946970
C	1.286432	2.761013	3.637454
C	1.586777	1.618569	2.753926
C	3.190180	0.107229	1.563188
C	4.541573	-0.220529	1.125787
C	4.502519	-1.511847	0.645202
C	3.109325	-1.943234	0.725202
C	2.599165	-3.127916	0.200030
H	3.320391	-3.819157	-0.222692
C	-2.237522	-2.923393	0.494358
H	-3.044854	-3.562443	0.150891
C	-1.889983	1.077436	3.185596
H	-2.580782	1.684224	3.758237
C	2.833220	1.274325	2.236455
H	3.648695	1.963698	2.432254
C	-1.212648	-0.581823	-2.898886
H	-0.754680	-0.286693	-1.952667
H	-0.563580	-0.286151	-3.728548
H	-1.348852	-1.668137	-2.911710
H	-2.183500	-0.090674	-3.017754
h	0.636750	-3.141790	3.778131
h	1.330893	-5.437600	-1.086400
h	-1.385634	-5.229423	-0.995023
h	-4.834372	-1.978097	1.207536
h	-4.659803	0.330271	2.835006
h	-0.713601	3.277026	4.549111
h	2.034843	3.509847	3.896675
h	5.381867	0.473545	1.141038
h	5.325650	-2.104582	0.246220

^{4}TS$_{H}$(III)

S	0.525982	-1.751749	3.766045
O	0.185534	0.066142	-0.089116
Fe	0.308854	-0.871704	1.437095
N	0.187080	-2.688703	0.496335
N	-1.711660	-0.897624	1.703457
N	0.459982	0.864018	2.490403
N	2.322706	-0.934792	1.258392
C	1.233201	-3.465820	0.016826
C	0.724218	-4.660572	-0.655370
C	-0.651876	-4.590175	-0.588499
C	-0.971603	-3.372624	0.148343
C	-2.619431	-1.810383	1.199697
C	-3.984460	-1.439305	1.564932

C	-3.895604	-0.294462	2.343219
C	-2.456191	0.025188	2.411018
C	-0.557699	1.485756	3.180481
C	-0.058022	2.655740	3.910309
C	1.286829	2.762001	3.616129
C	1.588985	1.622805	2.724640
C	3.190573	0.104565	1.536313
C	4.542959	-0.229609	1.103278
C	4.496071	-1.515477	0.609749
C	3.097326	-1.935617	0.676244
C	2.580277	-3.109798	0.134765
H	3.301726	-3.801675	-0.287377
C	-2.256635	-2.951112	0.480470
H	-3.064047	-3.605257	0.165286
C	-1.887834	1.084892	3.125732
H	-2.579271	1.688391	3.701944
C	2.837868	1.270686	2.216337
H	3.657550	1.951949	2.423858
C	-1.083315	-0.657192	-2.218983
H	-0.370543	-0.333572	-0.934088
H	-0.388527	-0.216128	-2.930901
H	-1.152272	-1.742019	-2.216861
H	-2.014433	-0.112771	-2.081699
h	0.637341	-3.126311	3.715799
h	1.321163	-5.437207	-1.133451
h	-1.398498	-5.262222	-1.011555
h	-4.849869	-2.002171	1.215196
h	-4.658731	0.324080	2.815562
h	-0.718093	3.275752	4.516905
h	2.038766	3.502293	3.889303
h	5.390479	0.455199	1.131822
h	5.318396	-2.112052	0.214848

^{4}IC(III)

S	0.529355	-1.758073	3.796365
O	0.200546	0.062711	-0.064086
Fe	0.326733	-0.880216	1.488371
N	0.199690	-2.683389	0.517789
N	-1.696947	-0.896450	1.731220
N	0.477034	0.863009	2.527390
N	2.338744	-0.938105	1.298981
C	1.245682	-3.464325	0.043274
C	0.735639	-4.653635	-0.638642
C	-0.640676	-4.575194	-0.584496
C	-0.960078	-3.358142	0.152998
C	-2.606875	-1.797653	1.210901
C	-3.972302	-1.422826	1.570385
C	-3.881976	-0.284683	2.358999
C	-2.441121	0.026997	2.438059
C	-0.541831	1.488408	3.210029
C	-0.045441	2.666477	3.930472
C	1.298647	2.774269	3.633581
C	1.602731	1.627611	2.751364
C	3.203583	0.106335	1.563808
C	4.553799	-0.223788	1.120270
C	4.508260	-1.511582	0.631793
C	3.111245	-1.936745	0.711222
C	2.593129	-3.110727	0.168195
H	3.314260	-3.802738	-0.254514
C	-2.245240	-2.931108	0.478806
H	-3.054067	-3.576497	0.149632
C	-1.872049	1.085811	3.154433
H	-2.564437	1.691889	3.726782
C	2.850786	1.275249	2.239885
H	3.669608	1.960279	2.439031
C	-1.209622	-0.680306	-2.674328
H	-0.309867	-0.418314	-0.759042
H	-0.347339	-0.264454	-3.181627
H	-1.326085	-1.754219	-2.585465
H	-2.008470	-0.017467	-2.366021
h	0.638428	-3.132629	3.741189
h	1.330973	-5.431261	-1.117122
h	-1.387935	-5.243678	-1.012046
h	-4.838046	-1.980312	1.212946
h	-4.645087	0.333292	2.832112
h	-0.707813	3.288531	4.532451
h	2.048958	3.519297	3.898219
h	5.397670	0.465865	1.138347
h	5.329312	-2.106751	0.232150

^{4}IC(IV)

S	0.490932	-1.775268	3.755990
O	0.219330	0.025796	-0.049046
Fe	0.333145	-0.884685	1.502912
N	0.214291	-2.675403	0.545268
N	-1.695368	-0.879723	1.733093
N	0.468383	0.836610	2.548155
N	2.343838	-0.948713	1.305723

C	1.270200	-3.466033	0.076972
C	0.749017	-4.643530	-0.603826
C	-0.628628	-4.554309	-0.558718
C	-0.953666	-3.341565	0.176291
C	-2.596853	-1.790212	1.207109
C	-3.962519	-1.414282	1.564234
C	-3.880647	-0.279659	2.357035
C	-2.444040	0.042391	2.447950
C	-0.559242	1.471010	3.224011
C	-0.053044	2.644074	3.931690
C	1.294737	2.745236	3.634527
C	1.604144	1.599561	2.762443
C	3.199608	0.105368	1.573566
C	4.547390	-0.223456	1.124755
C	4.507541	-1.513952	0.642061
C	3.116159	-1.949217	0.723327
C	2.614345	-3.133703	0.197556
H	3.334372	-3.831136	-0.214233
C	-2.242852	-2.922200	0.480654
H	-3.046800	-3.569360	0.147593
C	-1.892201	1.094259	3.169674
H	-2.582874	1.706067	3.735329
C	2.855651	1.265146	2.256422
H	3.671652	1.949384	2.462460
C	-1.216674	-0.646103	-2.660248
H	-0.305637	-0.409006	-0.763513
H	-0.374925	-0.264609	-3.226486
H	-1.331877	-1.712929	-2.504364
H	-2.011902	0.033414	-2.378945
h	0.625606	-3.147634	3.702881
h	1.338049	-5.423624	-1.086071
h	-1.375009	-5.219093	-0.993509
h	-4.825786	-1.972796	1.202436
h	-4.648860	0.331749	2.830423
h	-0.711174	3.277169	4.526772
h	2.041281	3.495732	3.894323
h	5.387569	0.470820	1.136868
h	5.329667	-2.107062	0.241566

^{4}TSreb(III)

S	0.506395	-1.771166	3.827997
O	-0.006735	-0.003654	-0.222075
Fe	0.263333	-0.874907	1.440765
N	0.163958	-2.688870	0.504532
N	-1.751338	-0.871499	1.730923
N	0.396908	0.882171	2.461975
N	2.277107	-0.938620	1.227411
C	1.200939	-3.483106	0.038770
C	0.679053	-4.668870	-0.644734
C	-0.694161	-4.566742	-0.606035
C	-1.002475	-3.337840	0.125781
C	-2.649484	-1.767816	1.188942
C	-4.018660	-1.410371	1.557259
C	-3.939219	-0.289037	2.372464
C	-2.502729	0.029461	2.461640
C	-0.599651	1.487817	3.203803
C	-0.082504	2.649768	3.927067
C	1.253450	2.766291	3.590148
C	1.534438	1.640250	2.677655
C	3.140247	0.110818	1.494852
C	4.497888	-0.228498	1.080958
C	4.459014	-1.523993	0.609744
C	3.061593	-1.947657	0.674791
C	2.548881	-3.135815	0.156521
H	3.269887	-3.836038	-0.252962
C	-2.282898	-2.893737	0.441812
H	-3.094723	-3.530488	0.102902
C	-1.930655	1.080048	3.183651
H	-2.613884	1.676400	3.776593
C	2.781091	1.282859	2.161217
H	3.600919	1.964524	2.367234
C	-0.674906	0.308387	-2.391553
H	-0.415868	0.864319	-0.010825
H	0.238011	0.753007	-2.765936
H	-0.828209	-0.755625	-2.501366
H	-1.528754	0.944303	-2.186199
h	0.635944	-3.143305	3.758734
h	1.272748	-5.451625	-1.116843
h	-1.446667	-5.226122	-1.038491
h	-4.880791	-1.966647	1.189354
h	-4.704542	0.317443	2.856745
h	-0.724639	3.262265	4.559980
h	2.008463	3.508680	3.848758
h	5.345169	0.456616	1.109226
h	5.284298	-2.119223	0.219011

^{4}P

S	0.446941	-1.818105	3.968528

O	-0.064903	0.495469	-0.312345
Fe	0.295102	-0.955373	1.610870
N	0.168029	-2.657587	0.526902
N	-1.748218	-0.861382	1.722545
N	0.402455	0.880907	2.501791
N	2.276714	-0.915785	1.247782
C	1.219972	-3.453546	0.061969
C	0.698448	-4.637276	-0.609525
C	-0.678831	-4.545929	-0.565274
C	-1.001661	-3.326549	0.161444
C	-2.650387	-1.771165	1.194708
C	-4.016158	-1.400503	1.551944
C	-3.936739	-0.268029	2.352349
C	-2.501351	0.054580	2.445690
C	-0.615480	1.495365	3.219327
C	-0.100536	2.644541	3.956642
C	1.248737	2.745597	3.658993
C	1.547041	1.625327	2.752086
C	3.139879	0.133115	1.539932
C	4.492257	-0.199146	1.109091
C	4.455319	-1.489130	0.621084
C	3.062162	-1.919849	0.683102
C	2.564754	-3.114833	0.175022
H	3.286290	-3.817469	-0.225956
C	-2.289771	-2.903762	0.466320
H	-3.093689	-3.552683	0.135909
C	-1.947766	1.108043	3.170778
H	-2.637611	1.706017	3.752709
C	2.798063	1.284298	2.241386
H	3.620179	1.955414	2.467248
C	-0.893860	0.171853	-1.468184
H	-0.435011	1.241101	0.204777
H	-0.882621	0.990105	-2.196061
H	-0.447518	-0.716276	-1.913572
H	-1.923167	-0.051564	-1.170242
h	0.601686	-3.183609	3.842826
h	1.291167	-5.419060	-1.084461
h	-1.424157	-5.213991	-0.996840
h	-4.877951	-1.961888	1.191075
h	-4.704702	0.335551	2.836074
h	-0.746204	3.261473	4.581600
h	2.004041	3.476966	3.946537
h	5.338062	0.487737	1.138609
h	5.280967	-2.079850	0.224320

Ethane reaction:

^{2}RC

S	0.556137	-1.737683	3.756505
O	0.149766	-0.030814	-0.061812
Fe	0.279930	-0.799641	1.398258
N	0.193132	-2.652899	0.571907
N	-1.744316	-0.834633	1.672789
N	0.399949	0.921774	2.469050
N	2.314006	-0.874072	1.286916
C	1.248412	-3.417906	0.091279
C	0.752322	-4.644122	-0.519080
C	-0.620964	-4.610994	-0.418991
C	-0.955835	-3.371348	0.266936
C	-2.634029	-1.773651	1.189324
C	-4.012838	-1.394271	1.491485
C	-3.951544	-0.213920	2.213209
C	-2.517558	0.111868	2.318090
C	-0.639375	1.575358	3.096410
C	-0.161033	2.760115	3.805302
C	1.199804	2.832964	3.585799
C	1.531648	1.672337	2.738724
C	3.189575	0.131244	1.659896
C	4.558329	-0.225952	1.300005
C	4.505710	-1.473617	0.712903
C	3.097700	-1.861664	0.698507
C	2.588143	-3.036277	0.159513
H	3.315609	-3.721897	-0.260433
C	-2.249391	-2.951347	0.552431
H	-3.043648	-3.631464	0.261390
C	-1.971886	1.183778	3.022243
H	-2.672593	1.797319	3.575874
C	2.806431	1.296964	2.320179
H	3.612552	1.975810	2.576419
C	-1.300275	-1.200801	-2.802134
H	-0.543647	-0.663985	-2.221631
H	-2.068439	-1.516967	-2.085845
H	-1.763376	-0.493030	-3.501603
C	-0.699542	-2.414021	-3.527860
H	-1.462968	-2.995481	-4.061985
H	-0.207054	-3.081435	-2.814869
H	0.051393	-2.112804	-4.268864
h	0.718985	-3.107262	3.710898
h	1.352309	-5.384168	-1.048620

h	-1.355390	-5.309618	-0.819751
h	-4.858858	-1.985219	1.140635
h	-4.727764	0.431090	2.624926
h	-0.838194	3.426687	4.339344
h	1.943231	3.564959	3.901341
h	5.440199	0.396020	1.453383
h	5.324063	-2.041876	0.270810

$^{2}TS_{H}$(III)

S	0.490454	-1.766100	3.753305
O	0.139880	-0.081615	-0.160900
Fe	0.179409	-0.936336	1.417804
N	0.021720	-2.774773	0.582591
N	-1.845054	-0.909965	1.660785
N	0.358852	0.842939	2.407918
N	2.209581	-1.022207	1.262621
C	1.062888	-3.571577	0.126056
C	0.543583	-4.792955	-0.476428
C	-0.829997	-4.725729	-0.398665
C	-1.141770	-3.482942	0.294644
C	-2.768939	-1.845097	1.229447
C	-4.129755	-1.424627	1.547738
C	-4.026624	-0.220934	2.226810
C	-2.583644	0.076684	2.291126
C	-0.664391	1.524443	3.027358
C	-0.158925	2.700761	3.737846
C	1.204621	2.734825	3.528303
C	1.508534	1.562522	2.682689
C	3.108358	-0.021579	1.583028
C	4.457717	-0.393292	1.161992
C	4.368975	-1.652497	0.607577
C	2.957508	-2.032099	0.668243
C	2.413376	-3.216962	0.185225
H	3.114828	-3.946968	-0.205721
C	-2.422135	-3.044888	0.608567
H	-3.230461	-3.726618	0.363704
C	-2.004573	1.156362	2.960313
H	-2.689063	1.794108	3.507538
C	2.770018	1.153291	2.253984
H	3.604855	1.802315	2.503014
C	-1.272274	-0.912943	-2.115176
H	-0.431801	-0.553494	-0.999764
H	-2.197753	-1.125382	-1.575656
H	-1.277502	0.056372	-2.619537
C	-0.678436	-2.069659	-2.878611
H	-1.287715	-2.309193	-3.767135
H	-0.633357	-2.977076	-2.273491
H	0.335088	-1.856911	-3.232742
h	0.663530	-3.134955	3.728271
h	1.144631	-5.531319	-1.007112
h	-1.574657	-5.380256	-0.851593
h	-4.996579	-2.010001	1.241110
h	-4.780713	0.450977	2.636630
h	-0.821672	3.383902	4.269026
h	1.967458	3.443573	3.850521
h	5.336185	0.246837	1.243198
h	5.151794	-2.230865	0.116912

^{2}IC(III)

S	0.520812	-1.748141	3.761022
O	0.131433	-0.035591	-0.153673
Fe	0.249377	-0.892113	1.457315
N	0.123398	-2.723635	0.568078
N	-1.779827	-0.900233	1.680139
N	0.391412	0.884554	2.438546
N	2.275927	-0.951101	1.293152
C	1.176170	-3.509041	0.120075
C	0.679101	-4.741046	-0.477831
C	-0.696252	-4.690499	-0.407835
C	-1.028043	-3.444390	0.270257
C	-2.687137	-1.834542	1.210920
C	-4.057207	-1.431809	1.515287
C	-3.976031	-0.238440	2.215805
C	-2.536612	0.070590	2.307864
C	-0.643187	1.547420	3.059260
C	-0.157757	2.731446	3.772497
C	1.204745	2.787592	3.565149
C	1.527936	1.620681	2.717564
C	3.158274	0.060567	1.620214
C	4.514756	-0.288995	1.204205
C	4.447598	-1.547670	0.644302
C	3.041920	-1.946493	0.694914
C	2.520141	-3.133471	0.192385
H	3.237470	-3.843703	-0.205425
C	-2.318021	-3.018096	0.571488
H	-3.116690	-3.702353	0.301041
C	-1.976568	1.156645	2.986960
H	-2.673190	1.782488	3.532860

C	2.796738	1.229320	2.292945
H	3.619723	1.890326	2.548867
C	-1.251449	-1.289166	-2.798829
H	-0.239312	-0.636246	-0.840902
H	-2.039785	-1.369607	-2.055157
H	-1.052469	-0.300617	-3.202949
C	-0.683636	-2.518037	-3.428245
H	-1.313189	-2.888614	-4.260076
H	-0.604940	-3.336038	-2.705353
H	0.314641	-2.345134	-3.847410
h	0.678398	-3.118671	3.726984
h	1.286995	-5.477020	-1.004018
h	-1.431931	-5.372635	-0.833902
h	-4.915210	-2.018198	1.186587
h	-4.742597	0.420331	2.623805
h	-0.831839	3.403489	4.303570
h	1.956951	3.507330	3.887994
h	5.387045	0.358621	1.292364
h	5.239100	-2.115023	0.154708

$^{2}TS_{H}(IV)$

S	0.440249	-1.769496	3.718923
O	0.134428	-0.095959	-0.110634
Fe	0.192365	-0.952872	1.427520
N	0.034859	-2.773983	0.601585
N	-1.837418	-0.903980	1.667996
N	0.363103	0.815120	2.427899
N	2.217339	-1.039616	1.253503
C	1.082767	-3.579629	0.144952
C	0.548681	-4.789280	-0.455961
C	-0.826423	-4.710811	-0.381258
C	-1.138526	-3.473126	0.313692
C	-2.757948	-1.844663	1.233913
C	-4.117379	-1.417132	1.547941
C	-4.016707	-0.213448	2.226587
C	-2.575680	0.088792	2.298930
C	-0.666987	1.512278	3.029953
C	-0.150538	2.681525	3.735244
C	1.218037	2.694449	3.546613
C	1.523487	1.520144	2.710161
C	3.111472	-0.037915	1.592231
C	4.458171	-0.408106	1.165085
C	4.370389	-1.664079	0.602770
C	2.962297	-2.049203	0.660949
C	2.430176	-3.242370	0.191569
H	3.129344	-3.976021	-0.193245
C	-2.421595	-3.042165	0.615325
H	-3.227799	-3.724492	0.370572
C	-2.009106	1.171442	2.959280
H	-2.690546	1.821661	3.493418
C	2.787133	1.120008	2.287725
H	3.623107	1.759924	2.551251
C	-1.227974	-0.888961	-2.070647
H	-0.455497	-0.559130	-1.033888
H	-2.162361	-1.100749	-1.545647
H	-1.243584	0.070344	-2.595436
C	-0.642050	-2.053476	-2.830817
H	-1.269715	-2.285732	-3.707206
H	-0.597011	-2.957582	-2.221443
H	0.366719	-1.847093	-3.200104
h	0.636038	-3.135381	3.699666
h	1.141975	-5.530991	-0.990688
h	-1.571267	-5.360510	-0.840786
h	-4.984935	-2.000669	1.239887
h	-4.772554	0.455124	2.638622
h	-0.809941	3.381082	4.248930
h	1.983310	3.395252	3.880226
h	5.335053	0.234264	1.245743
h	5.154264	-2.240322	0.111292

$^{2}IC(IV)$

S	0.450451	-1.769763	3.738852
O	0.116220	-0.062842	-0.108788
Fe	0.231239	-0.902956	1.480288
N	0.076263	-2.713227	0.600971
N	-1.805781	-0.863075	1.712237
N	0.392207	0.843206	2.476479
N	2.254255	-0.999945	1.298612
C	1.124539	-3.528939	0.158790
C	0.589667	-4.736101	-0.443753
C	-0.786778	-4.645961	-0.386767
C	-1.098758	-3.403778	0.297803
C	-2.721426	-1.789759	1.241972
C	-4.084701	-1.365853	1.551116
C	-3.989006	-0.176716	2.254606
C	-2.547641	0.120983	2.347334
C	-0.640177	1.538238	3.083141
C	-0.124270	2.708935	3.781519

C	1.244836	2.725414	3.588738	C	-2.778780	-1.745506	1.271669
C	1.552306	1.554420	2.752419	C	-4.142385	-1.323857	1.581014
C	3.145365	0.006433	1.628691	C	-4.048173	-0.137132	2.294367
C	4.491520	-0.360030	1.197361	C	-2.606646	0.157677	2.389854
C	4.407162	-1.619567	0.642108	C	-0.696374	1.584154	3.122551
C	3.000572	-2.009309	0.704865	C	-0.164321	2.737501	3.837246
C	2.472809	-3.200497	0.225992	C	1.205006	2.739509	3.641297
H	3.173173	-3.934987	-0.154788	C	1.495607	1.578816	2.780563
C	-2.382881	-2.972293	0.597336	C	3.075200	0.007999	1.639293
H	-3.189047	-3.648245	0.335015	C	4.429217	-0.376719	1.241368
C	-1.982836	1.199092	3.015385	C	4.339961	-1.626392	0.662001
H	-2.663893	1.850215	3.548778	C	2.923896	-1.986476	0.674417
C	2.816579	1.164517	2.321810	C	2.387931	-3.163537	0.167629
H	3.648741	1.812060	2.578241	H	3.086032	-3.898033	-0.218506
C	-1.234249	-1.214641	-2.656514	C	-2.445074	-2.921586	0.603904
H	-0.194127	-0.635967	-0.855167	H	-3.258742	-3.590419	0.343809
H	-2.050447	-1.294648	-1.943005	C	-2.038655	1.236755	3.063847
H	-1.018418	-0.226157	-3.054369	H	-2.717713	1.877771	3.613289
C	-0.689268	-2.444423	-3.302838	C	2.754748	1.161097	2.351867
H	-1.303125	-2.759504	-4.167852	H	3.598929	1.782343	2.635673
H	-0.674021	-3.287127	-2.605651	C	-0.702661	0.586371	-1.524050
H	0.330014	-2.301240	-3.680276	H	-0.259452	1.202103	0.386901
h	0.646759	-3.135169	3.700424	H	-1.516708	1.318504	-1.455492
h	1.181815	-5.491350	-0.960501	H	0.078406	0.989982	-2.180313
h	-1.531836	-5.301142	-0.838090	C	-1.218099	-0.737594	-2.059048
h	-4.950476	-1.941856	1.224433	H	-1.598599	-0.592877	-3.078454
h	-4.747400	0.486763	2.670179	H	-2.024997	-1.128188	-1.434487
h	-0.784663	3.411611	4.289649	H	-0.424673	-1.489815	-2.085362
h	2.007216	3.429495	3.922074	h	0.643564	-3.130168	3.671322
h	5.366041	0.286331	1.271493	h	1.082184	-5.423690	-1.072165
h	5.189437	-2.195693	0.147952	h	-1.629933	-5.234059	-0.910288
				h	-5.007216	-1.898930	1.250223
^{2}P				h	-4.805947	0.519591	2.721638
S	0.417867	-1.770734	3.744439	h	-0.819166	3.437453	4.356199
O	-0.116778	0.415229	-0.180925	h	1.980558	3.424443	3.984006
Fe	0.170825	-0.933558	1.578800	h	5.315752	0.249936	1.338460
N	0.005291	-2.671974	0.563841	h	5.125440	-2.202465	0.172890
N	-1.861012	-0.820563	1.745913				
N	0.322586	0.896557	2.473477	^{4}RC			
N	2.169429	-0.971725	1.257416	S	0.555122	-1.735778	3.750735
C	1.036125	-3.479367	0.086503	O	0.142503	-0.035606	-0.054840
C	0.491762	-4.673066	-0.546778	Fe	0.284629	-0.805572	1.406215
C	-0.878569	-4.580434	-0.467240	N	0.193916	-2.652041	0.571224
C	-1.170548	-3.352175	0.263874	N	-1.743626	-0.834733	1.672469

N	0.401081	0.920590	2.470712
N	2.314003	-0.874488	1.286884
C	1.248780	-3.418448	0.090918
C	0.752084	-4.644003	-0.519282
C	-0.620994	-4.610647	-0.418944
C	-0.955945	-3.370846	0.266772
C	-2.634089	-1.773383	1.189039
C	-4.012720	-1.394011	1.491268
C	-3.951483	-0.213866	2.212942
C	-2.517262	0.111686	2.318472
C	-0.638926	1.574759	3.096983
C	-0.160858	2.759920	3.805312
C	1.200144	2.833083	3.586051
C	1.531967	1.672391	2.739211
C	3.189588	0.131185	1.660313
C	4.558195	-0.226201	1.300192
C	4.505278	-1.473991	0.713231
C	3.097768	-1.862427	0.699267
C	2.588381	-3.037103	0.159871
H	3.315949	-3.722586	-0.259953
C	-2.249606	-2.951111	0.552186
H	-3.043995	-3.631286	0.261604
C	-1.971711	1.183378	3.022822
H	-2.672493	1.797288	3.576187
C	2.806908	1.296974	2.320420
H	3.613074	1.975796	2.576477
C	-1.299807	-1.200976	-2.802763
H	-0.543244	-0.664705	-2.221859
H	-2.068426	-1.516853	-2.086764
H	-1.762228	-0.492815	-3.502271
C	-0.699419	-2.414231	-3.528494
H	-1.463081	-2.995023	-4.062948
H	-0.207735	-3.082156	-2.815459
H	0.051972	-2.113406	-4.269225
h	0.718514	-3.105391	3.708171
h	1.352055	-5.384165	-1.048679
h	-1.355339	-5.309449	-0.819542
h	-4.858911	-1.984892	1.140716
h	-4.727616	0.431189	2.624751
h	-0.838110	3.426640	4.339054
h	1.943506	3.565268	3.901303
h	5.439995	0.395951	1.453239
h	5.323765	-2.042114	0.271212

$^{4}TS_{H}(III)$

S	0.494128	-1.760563	3.752146
O	0.065832	-0.093964	-0.169372
Fe	0.193348	-0.922575	1.417558
N	0.031682	-2.773105	0.585314
N	-1.840474	-0.907837	1.680553
N	0.364482	0.851963	2.402105
N	2.210663	-1.009792	1.247438
C	1.068834	-3.570873	0.128142
C	0.548328	-4.792722	-0.472158
C	-0.825570	-4.721973	-0.393814
C	-1.132735	-3.477299	0.299599
C	-2.762075	-1.841023	1.242212
C	-4.124489	-1.419094	1.554587
C	-4.022380	-0.215127	2.233800
C	-2.579228	0.079747	2.302479
C	-0.658865	1.531049	3.028996
C	-0.150436	2.702694	3.744832
C	1.212901	2.735381	3.535690
C	1.514069	1.569082	2.681140
C	3.110893	-0.011157	1.569685
C	4.460690	-0.385687	1.154839
C	4.372316	-1.646781	0.604120
C	2.960930	-2.025303	0.660904
C	2.419829	-3.214127	0.185082
H	3.122775	-3.945292	-0.201073
C	-2.413291	-3.037904	0.616756
H	-3.222167	-3.717947	0.368290
C	-1.998356	1.164020	2.965881
H	-2.681740	1.803725	3.512302
C	2.773569	1.163200	2.243011
H	3.609083	1.811526	2.491222
C	-1.287098	-0.957348	-2.164839
H	-0.478032	-0.587534	-1.018847
H	-2.232461	-1.168146	-1.660144
H	-1.274670	0.012976	-2.667291
C	-0.672379	-2.114080	-2.911912
H	-1.265204	-2.368702	-3.807342
H	-0.625480	-3.015845	-2.297965
H	0.344646	-1.893113	-3.250807
h	0.662773	-3.130026	3.730344
h	1.148001	-5.532266	-1.002756
h	-1.571389	-5.375134	-0.846806
h	-4.991499	-2.003046	1.245783

h	-4.776343	0.458440	2.641126
h	-0.812037	3.385537	4.277821
h	1.978117	3.437772	3.866078
h	5.339689	0.253390	1.238546
h	5.156012	-2.225848	0.115685

^{4}IC(III)

S	0.497132	-1.759365	3.755791
O	-0.004480	-0.063581	-0.137107
Fe	0.210432	-0.901061	1.475420
N	0.086811	-2.732930	0.574891
N	-1.815100	-0.888697	1.729575
N	0.351296	0.876746	2.442596
N	2.230799	-0.978303	1.265192
C	1.127601	-3.537886	0.129949
C	0.609819	-4.754416	-0.480592
C	-0.765476	-4.672958	-0.423033
C	-1.074718	-3.425306	0.265492
C	-2.721934	-1.811628	1.237531
C	-4.093488	-1.404977	1.539738
C	-4.010550	-0.221559	2.254584
C	-2.570087	0.076869	2.360421
C	-0.666860	1.542844	3.088205
C	-0.162098	2.726494	3.787804
C	1.194841	2.780551	3.547450
C	1.497149	1.611531	2.693553
C	3.112675	0.038217	1.581686
C	4.469459	-0.316791	1.172107
C	4.404335	-1.585397	0.631315
C	3.000603	-1.985028	0.687735
C	2.475993	-3.180028	0.204344
H	3.189176	-3.903843	-0.177202
C	-2.359898	-2.985618	0.579081
H	-3.165098	-3.658195	0.298688
C	-2.002667	1.156762	3.042640
H	-2.690518	1.782535	3.599937
C	2.756354	1.215086	2.246850
H	3.583894	1.878008	2.483528
C	-1.171718	-1.308434	-2.824637
H	0.107043	-0.703688	-0.876349
H	-1.893863	-1.352350	-2.015633
H	-0.942019	-0.324916	-3.225034
C	-0.708820	-2.556370	-3.501268
H	-1.414078	-2.896395	-4.284004
H	-0.617729	-3.381405	-2.787350
H	0.262665	-2.426429	-3.994441
h	0.672887	-3.127714	3.722979
h	1.212610	-5.503302	-0.994284
h	-1.511418	-5.332575	-0.866362
h	-4.952160	-1.984414	1.200618
h	-4.774098	0.442005	2.660472
h	-0.825777	3.402573	4.326797
h	1.953732	3.500941	3.852719
h	5.340212	0.333922	1.252285
h	5.195331	-2.158050	0.147105

^{4}IC(IV)

S	0.446686	-1.770367	3.719866
O	0.074621	-0.076015	-0.136470
Fe	0.226136	-0.899891	1.466165
N	0.089852	-2.713985	0.582841
N	-1.811908	-0.883885	1.702765
N	0.368866	0.845555	2.450320
N	2.249765	-0.978785	1.275011
C	1.144935	-3.523538	0.147797
C	0.620683	-4.735478	-0.454285
C	-0.756416	-4.651741	-0.408044
C	-1.079537	-3.410031	0.272812
C	-2.718872	-1.812071	1.218412
C	-4.086538	-1.401096	1.529178
C	-4.000911	-0.218307	2.243466
C	-2.561804	0.087634	2.344180
C	-0.666416	1.521459	3.077376
C	-0.159056	2.699889	3.767953
C	1.204963	2.746946	3.542863
C	1.521257	1.578255	2.707687
C	3.131193	0.038516	1.596505
C	4.482463	-0.320462	1.174876
C	4.411110	-1.586066	0.630912
C	3.007763	-1.987808	0.693180
C	2.491151	-3.185659	0.219281
H	3.199338	-3.915657	-0.155913
C	-2.368832	-2.987035	0.566363
H	-3.168966	-3.665767	0.291511
C	-2.004423	1.162346	3.024820
H	-2.689497	1.795399	3.574410
C	2.788639	1.201510	2.274856
H	3.612670	1.861532	2.524958

C	-1.233579	-1.291367	-2.761114
H	-0.105224	-0.691718	-0.886038
H	-1.985344	-1.389311	-1.982542
H	-1.060963	-0.296875	-3.164325
C	-0.706756	-2.508726	-3.446007
H	-1.376299	-2.846324	-4.260138
H	-0.616520	-3.347043	-2.749109
H	0.275721	-2.340056	-3.902881
h	0.641638	-3.136039	3.684084
h	1.220171	-5.487196	-0.967705
h	-1.498157	-5.312962	-0.856011
h	-4.947293	-1.980105	1.194640
h	-4.764117	0.441516	2.656038
h	-0.818961	3.387454	4.296959
h	1.957026	3.474574	3.847861
h	5.351378	0.333661	1.246826
h	5.197636	-2.161235	0.142420

^{4}TSreb(III)

S	0.497819	-1.780178	3.833647
O	-0.035181	0.076469	-0.140103
Fe	0.197078	-0.852185	1.498124
N	0.037718	-2.652467	0.574780
N	-1.840615	-0.797827	1.765499
N	0.361928	0.913969	2.500982
N	2.215574	-0.960893	1.304774
C	1.059339	-3.463999	0.110846
C	0.518116	-4.654794	-0.538059
C	-0.851240	-4.548968	-0.482100
C	-1.139711	-3.312361	0.240704
C	-2.756579	-1.697526	1.262343
C	-4.122199	-1.286033	1.580355
C	-4.024585	-0.117151	2.322543
C	-2.582101	0.164077	2.426603
C	-0.648599	1.590971	3.156212
C	-0.126311	2.763861	3.852312
C	1.235448	2.792377	3.618769
C	1.520383	1.625590	2.761158
C	3.119919	0.033450	1.646312
C	4.472685	-0.353475	1.247862
C	4.382848	-1.614384	0.693629
C	2.966841	-1.977026	0.725068
C	2.415112	-3.145781	0.208388
H	3.110595	-3.879572	-0.185833
C	-2.410839	-2.865607	0.573573
H	-3.228334	-3.522343	0.291374
C	-1.992825	1.225974	3.115315
H	-2.666490	1.862976	3.677198
C	2.779543	1.207133	2.318830
H	3.616853	1.850410	2.574650
C	-0.797413	0.643101	-2.248304
H	-0.331968	0.975784	0.122752
H	-1.400414	1.488945	-1.925618
H	0.188036	0.863935	-2.641995
C	-1.457919	-0.662762	-2.530030
H	-2.065477	-0.630621	-3.452935
H	-2.125088	-0.945924	-1.707983
H	-0.726274	-1.469878	-2.637247
h	0.684807	-3.145421	3.759527
h	1.109416	-5.409203	-1.056998
h	-1.603898	-5.199116	-0.928059
h	-4.987042	-1.854212	1.237886
h	-4.778747	0.542330	2.751951
h	-0.784408	3.454837	4.379120
h	2.005232	3.495756	3.936192
h	5.358461	0.275496	1.336534
h	5.163478	-2.194655	0.201725

^{4}P

S	0.453997	-1.828077	3.939519
O	-0.191264	0.558719	-0.380652
Fe	0.185117	-0.962400	1.611687
N	0.011906	-2.681805	0.590255
N	-1.859788	-0.833701	1.724322
N	0.336495	0.886750	2.451863
N	2.182604	-0.966596	1.254661
C	1.049169	-3.487254	0.114062
C	0.507747	-4.673319	-0.526616
C	-0.865810	-4.580420	-0.458638
C	-1.166626	-3.358850	0.268925
C	-2.781760	-1.754929	1.252909
C	-4.141977	-1.330669	1.564328
C	-4.042610	-0.142734	2.275612
C	-2.600677	0.148592	2.368219
C	-0.687571	1.573357	3.095655
C	-0.160942	2.727522	3.809551
C	1.209149	2.737691	3.610703
C	1.505044	1.583019	2.749988

C	3.089176	0.022111	1.616296
C	4.439859	-0.365919	1.219418
C	4.349936	-1.623335	0.656776
C	2.936171	-1.988459	0.683079
C	2.400968	-3.171434	0.192176
H	3.097587	-3.907958	-0.191647
C	-2.445838	-2.932336	0.592362
H	-3.255912	-3.602111	0.325297
C	-2.030069	1.226988	3.038563
H	-2.707456	1.870047	3.586909
C	2.766940	1.178317	2.317969
H	3.606801	1.806598	2.596997
C	-0.814930	0.708726	-1.701514
H	-0.384087	1.316441	0.207906
H	-1.650289	1.417034	-1.634578
H	-0.067415	1.112866	-2.397128
C	-1.301221	-0.650654	-2.177869
H	-1.714271	-0.571076	-3.191035
H	-2.071929	-1.042410	-1.508419
H	-0.478024	-1.371690	-2.187552
h	0.661687	-3.187423	3.823812
h	1.097927	-5.422257	-1.054674
h	-1.612195	-5.234657	-0.909138
h	-5.009114	-1.905675	1.239505
h	-4.797695	0.514648	2.706613
h	-0.815240	3.422651	4.335628
h	1.980348	3.424466	3.959499
h	5.327580	0.258685	1.318862
h	5.133576	-2.202020	0.167798

Propane reaction:

^{2}RC

S	0.477868	-1.704587	3.917059
O	0.324488	-0.044862	0.050856
Fe	0.395370	-0.816729	1.509553
N	0.360050	-2.666332	0.635111
N	-1.637263	-0.868935	1.705748
N	0.459487	0.910998	2.567417
N	2.430624	-0.868241	1.457173
C	1.434466	-3.390663	0.135327
C	0.970407	-4.585828	-0.565922
C	-0.405230	-4.583113	-0.470455
C	-0.772137	-3.380979	0.269103
C	-2.496399	-1.819096	1.189612
C	-3.889681	-1.463463	1.461508
C	-3.867644	-0.291332	2.199894
C	-2.441791	0.064285	2.330944
C	-0.609293	1.574381	3.130396
C	-0.168172	2.779548	3.830767
C	1.202364	2.846813	3.680232
C	1.575394	1.672385	2.872951
C	3.279592	0.156041	1.835370
C	4.660203	-0.165798	1.487934
C	4.640135	-1.416101	0.908168
C	3.241644	-1.834786	0.872406
C	2.765420	-2.998966	0.281102
H	3.520966	-3.659147	-0.129579
C	-2.077736	-2.978335	0.538216
H	-2.859360	-3.654341	0.207400
C	-1.934282	1.165655	3.018531
H	-2.658866	1.794004	3.522099
C	2.864969	1.312489	2.492551
H	3.656742	1.999024	2.771051
C	-1.662348	0.831080	-3.563200
H	-2.001450	1.714597	-3.007752
H	-2.446179	0.572038	-4.288710
H	-0.767106	1.119558	-4.129586
C	-1.355347	-0.332906	-2.606822
H	-2.274140	-0.621768	-2.071753
H	-0.659247	0.002593	-1.831362
C	-0.759199	-1.572812	-3.293703
H	0.146035	-1.304509	-3.853299
H	-1.465693	-2.034134	-3.998426
H	-0.480199	-2.333420	-2.556176
h	0.647550	-3.072972	3.861575
h	1.603851	-5.302814	-1.088173
h	-1.123792	-5.296479	-0.873994
h	-4.723284	-2.053830	1.081193
h	-4.666536	0.322469	2.615932
h	-0.876457	3.465321	4.295648
h	1.932747	3.582022	4.017983
h	5.524956	0.482006	1.631521
h	5.481609	-1.983708	0.510916

^{2}TS$_{H}$(III)

S	0.473347	-1.691977	3.847869
O	0.327859	0.059766	-0.036675
Fe	0.341265	-0.862911	1.485885

N	0.296613	-2.679521	0.561339	h	-0.937739	3.450826	4.233707
N	-1.689279	-0.915531	1.647940	h	1.876695	3.558379	3.996123
N	0.415717	0.901673	2.506799	h	5.479940	0.464035	1.600755
N	2.382000	-0.876166	1.406682	h	5.436189	-1.994620	0.469162
C	1.380190	-3.397639	0.068751				
C	0.927463	-4.609719	-0.611961	$^{2}TS_{H}(IV)$			
C	-0.447467	-4.631002	-0.502131	S	0.458300	-1.696660	3.807024
C	-0.828394	-3.428415	0.228652	O	0.321365	0.047004	0.027687
C	-2.553651	-1.884451	1.170813	Fe	0.349122	-0.876936	1.495585
C	-3.941485	-1.533200	1.465424	N	0.309085	-2.679687	0.582549
C	-3.913632	-0.344748	2.179828	N	-1.683865	-0.913363	1.661439
C	-2.487275	0.025346	2.274848	N	0.414310	0.877380	2.529835
C	-0.659445	1.564199	3.055077	N	2.386240	-0.891568	1.403618
C	-0.226115	2.768957	3.768184	C	1.398735	-3.405475	0.090860
C	1.146127	2.831606	3.640963	C	0.933160	-4.606307	-0.592464
C	1.527602	1.656175	2.834120	C	-0.443401	-4.616211	-0.488836
C	3.232418	0.140179	1.800154	C	-0.825395	-3.417153	0.241682
C	4.614674	-0.182012	1.452414	C	-2.542844	-1.882342	1.172152
C	4.592690	-1.426010	0.860645	C	-3.929949	-1.525805	1.459803
C	3.190335	-1.839020	0.814406	C	-3.905951	-0.342551	2.182960
C	2.710756	-2.997581	0.214585	C	-2.482948	0.030279	2.292048
H	3.467912	-3.657497	-0.194357	C	-0.666630	1.548381	3.068765
C	-2.134881	-3.050040	0.527168	C	-0.223603	2.751616	3.769884
H	-2.911466	-3.748022	0.230840	C	1.151267	2.804317	3.648304
C	-1.980095	1.143664	2.939895	C	1.534301	1.625532	2.852412
H	-2.707989	1.772308	3.439162	C	3.230594	0.131020	1.807111
C	2.820750	1.289994	2.470559	C	4.610651	-0.189822	1.453815
H	3.615051	1.967169	2.765607	C	4.592154	-1.434231	0.862275
C	-1.271985	0.781347	-2.628271	C	3.194148	-1.854653	0.814806
H	-1.841259	1.374862	-1.904374	C	2.727713	-3.022333	0.228030
H	-1.864845	0.719117	-3.557429	H	3.483529	-3.685728	-0.174464
H	-0.351033	1.326280	-2.867641	C	-2.133115	-3.044619	0.525893
C	-0.955797	-0.599960	-2.094814	H	-2.908432	-3.737820	0.219792
H	-1.821211	-1.141747	-1.697979	C	-1.988479	1.146621	2.956383
H	-0.284170	-0.332823	-0.929249	H	-2.714201	1.780789	3.449687
C	0.003438	-1.445192	-2.902779	C	2.829174	1.269205	2.491546
H	0.966659	-0.933976	-3.018095	H	3.623091	1.941410	2.795354
H	-0.390095	-1.626407	-3.917462	C	-1.282237	0.796965	-2.626649
H	0.184877	-2.418761	-2.438651	H	-1.850654	1.396465	-1.907330
h	0.637274	-3.061276	3.797925	H	-1.887397	0.700738	-3.543168
h	1.565496	-5.324891	-1.131103	H	-0.372286	1.347519	-2.892463
h	-1.154909	-5.363090	-0.891542	C	-0.943804	-0.574406	-2.067985
h	-4.779020	-2.136990	1.116083	H	-1.818620	-1.124587	-1.700296
h	-4.709406	0.264319	2.608603	H	-0.341483	-0.339805	-0.996275

C	0.001674	-1.425455	-2.895993
H	0.949595	-0.902445	-3.066150
H	-0.438916	-1.637831	-3.883190
H	0.217372	-2.382808	-2.413454
h	0.630119	-3.065277	3.765652
h	1.565467	-5.325543	-1.112996
h	-1.152383	-5.344281	-0.882948
h	-4.766599	-2.124951	1.100488
h	-4.704697	0.260681	2.614450
h	-0.931807	3.445073	4.223351
h	1.881172	3.534146	3.998526
h	5.473901	0.460309	1.595926
h	5.437072	-2.001383	0.471740

^{2}IC(III)

S	0.481651	-1.695894	3.882800
O	0.328389	0.035274	-0.060003
Fe	0.376704	-0.846937	1.529957
N	0.326836	-2.670996	0.598518
N	-1.661939	-0.897776	1.678046
N	0.444767	0.916487	2.539020
N	2.409627	-0.858679	1.439470
C	1.407351	-3.385078	0.100054
C	0.955988	-4.594019	-0.586764
C	-0.419509	-4.616218	-0.475340
C	-0.798510	-3.415176	0.259753
C	-2.526607	-1.861483	1.189452
C	-3.916166	-1.503869	1.469600
C	-3.888565	-0.316105	2.185867
C	-2.461330	0.045458	2.294926
C	-0.631290	1.578995	3.086595
C	-0.199357	2.784792	3.799258
C	1.172587	2.849080	3.670806
C	1.553737	1.674536	2.862592
C	3.259489	0.159535	1.822343
C	4.641103	-0.161387	1.471264
C	4.619745	-1.409519	0.888794
C	3.217517	-1.824014	0.848051
C	2.738700	-2.982835	0.248946
H	3.497055	-3.642148	-0.159315
C	-2.105600	-3.030221	0.552667
H	-2.883626	-3.724430	0.250656
C	-1.952235	1.161599	2.964551
H	-2.681220	1.793189	3.458636
C	2.845931	1.312732	2.488783
H	3.639468	1.994079	2.776463
C	-1.330271	0.761195	-2.956040
H	-1.801012	1.394282	-2.194717
H	-1.893307	0.913674	-3.896894
H	-0.315168	1.138832	-3.131744
C	-1.307758	-0.677705	-2.540216
H	-2.158310	-1.066199	-1.978998
H	-0.246330	-0.407544	-0.728487
C	-0.335385	-1.657590	-3.119549
H	0.644167	-1.189921	-3.276972
H	-0.666277	-2.044725	-4.102304
H	-0.196931	-2.530947	-2.473210
h	0.637282	-3.066227	3.834705
h	1.596964	-5.302076	-1.111999
h	-1.129236	-5.344760	-0.867232
h	-4.753099	-2.102891	1.110739
h	-4.684464	0.295943	2.610142
h	-0.913195	3.466838	4.261118
h	1.901850	3.578854	4.022476
h	5.505307	0.487491	1.613306
h	5.462245	-1.978250	0.495342

^{2}IC(IV)

S	0.457869	-1.697532	3.812229
O	0.294805	0.027117	-0.024902
Fe	0.371693	-0.838891	1.529031
N	0.325537	-2.647592	0.599729
N	-1.670199	-0.872838	1.680388
N	0.431924	0.900641	2.556448
N	2.402481	-0.863689	1.429813
C	1.413588	-3.375063	0.108047
C	0.944914	-4.570529	-0.582086
C	-0.432624	-4.575207	-0.481460
C	-0.811474	-3.376609	0.252178
C	-2.527691	-1.837875	1.180174
C	-3.915932	-1.477702	1.460338
C	-3.892649	-0.298995	2.191500
C	-2.470054	0.069498	2.310491
C	-0.649900	1.573170	3.096141
C	-0.205179	2.774872	3.795524
C	1.170089	2.828523	3.669591
C	1.552089	1.652177	2.871991
C	3.246390	0.162186	1.821647

C	4.625463	-0.160545	1.466839	C	-2.523006	-1.949589	1.134276
C	4.606347	-1.409765	0.885058	C	-3.909614	-1.601725	1.437572
C	3.208187	-1.830908	0.842995	C	-3.885549	-0.410924	2.149214
C	2.743345	-2.999185	0.256212	C	-2.462371	-0.025992	2.233586
H	3.499337	-3.664892	-0.142079	C	-0.645912	1.518797	2.980203
C	-2.119159	-2.998993	0.531896	C	-0.208056	2.718666	3.696314
H	-2.896457	-3.686619	0.218801	C	1.163887	2.788706	3.560084
C	-1.973970	1.180119	2.981782	C	1.547243	1.625594	2.739486
H	-2.698005	1.816088	3.474817	C	3.246981	0.141288	1.680308
C	2.846767	1.302390	2.503477	C	4.625946	-0.201507	1.361185
H	3.639921	1.978615	2.800288	C	4.603252	-1.453957	0.781801
C	-1.294347	0.773791	-2.870491	C	3.203916	-1.862749	0.710883
H	-1.841488	1.362955	-2.125039	C	2.740981	-3.050515	0.155091
H	-1.837767	0.877820	-3.828698	H	3.502798	-3.718434	-0.230227
H	-0.308886	1.233300	-3.015144	C	-2.109830	-3.121236	0.501686
C	-1.168611	-0.663018	-2.463265	H	-2.884405	-3.822961	0.211690
H	-2.025269	-1.137004	-1.982404	C	-1.964990	1.099702	2.886501
H	-0.269244	-0.361276	-0.750656	H	-2.689212	1.722795	3.397038
C	-0.108264	-1.545097	-3.046682	C	2.843542	1.280114	2.366516
H	0.871594	-1.050459	-3.031243	H	3.637834	1.949401	2.677595
H	-0.317560	-1.788040	-4.105538	C	-1.184164	0.939725	-2.075577
H	-0.023168	-2.495918	-2.511548	H	-1.616832	1.523557	-1.258058
h	0.631202	-3.065841	3.767159	H	-1.969169	0.729453	-2.812586
h	1.577304	-5.288123	-1.104780	H	-0.413698	1.541164	-2.574059
h	-1.144242	-5.301444	-0.874202	C	-0.593925	-0.366753	-1.551525
h	-4.752548	-2.072646	1.094030	H	-1.373053	-0.980541	-1.097713
h	-4.691617	0.304555	2.622130	H	1.236987	0.062531	-0.675736
h	-0.912927	3.470112	4.246966	C	0.164670	-1.157453	-2.615585
h	1.898980	3.559605	4.019312	H	0.986936	-0.560226	-3.032764
h	5.487667	0.492549	1.601525	H	-0.509138	-1.412388	-3.441883
h	5.449741	-1.977765	0.492465	H	0.576252	-2.084301	-2.208468
				h	0.627158	-3.056454	3.733278
^{2}P				h	1.588116	-5.364854	-1.201193
S	0.483658	-1.684177	3.757989	h	-1.127662	-5.420236	-0.929093
O	0.305309	-0.062170	-0.404002	h	-4.748068	-2.208602	1.095867
Fe	0.371399	-0.950338	1.505640	h	-4.681517	0.186310	2.593978
N	0.326405	-2.748448	0.536033	h	-0.916183	3.395330	4.174591
N	-1.663193	-0.961683	1.593499	h	1.892290	3.516940	3.916697
N	0.433208	0.869247	2.408159	h	5.495797	0.434057	1.526967
N	2.387198	-0.866704	1.251212	h	5.452757	-2.030476	0.415695
C	1.413898	-3.459040	0.032784				
C	0.954495	-4.667172	-0.653625	^{4}RC			
C	-0.419500	-4.691080	-0.535515	S	0.482903	-1.699089	3.904420
C	-0.801685	-3.494348	0.205718	O	0.323348	-0.048126	0.057358

Fe	0.397330	-0.820466	1.517572	h	-4.667706	0.323392	2.614923
N	0.359159	-2.666881	0.636864	h	-0.877222	3.465272	4.297121
N	-1.638000	-0.868580	1.706118	h	1.932387	3.582175	4.019438
N	0.459608	0.910665	2.569766	h	5.524382	0.482089	1.630754
N	2.429696	-0.869115	1.458996	h	5.481275	-1.984448	0.512776
C	1.433645	-3.391506	0.136665				
C	0.969195	-4.585978	-0.566346	^4TS_H(III)			
C	-0.406495	-4.583545	-0.470772	S	0.478129	-1.688454	3.844975
C	-0.773297	-3.381188	0.269512	O	0.253595	0.034327	-0.074039
C	-2.497025	-1.818644	1.189250	Fe	0.351182	-0.832924	1.479659
C	-3.890439	-1.462737	1.461068	N	0.304283	-2.671558	0.565112
C	-3.868611	-0.290491	2.199397	N	-1.688738	-0.903476	1.665646
C	-2.442587	0.064960	2.331114	N	0.417011	0.920155	2.496269
C	-0.609771	1.574081	3.132246	N	2.380609	-0.850790	1.386696
C	-0.168747	2.779702	3.832230	C	1.382924	-3.387311	0.066958
C	1.201948	2.847064	3.681596	C	0.929559	-4.598923	-0.614064
C	1.575348	1.672105	2.875374	C	-0.445586	-4.618866	-0.499983
C	3.279184	0.155423	1.837216	C	-0.821379	-3.415945	0.234348
C	4.659836	-0.166374	1.488894	C	-2.549670	-1.872887	1.184489
C	4.639602	-1.416991	0.909820	C	-3.939627	-1.522276	1.473458
C	3.241095	-1.835891	0.874300	C	-3.914421	-0.332170	2.185561
C	2.764890	-2.999978	0.282513	C	-2.488107	0.037017	2.283771
H	3.520561	-3.659707	-0.128085	C	-0.657992	1.577422	3.057416
C	-2.078529	-2.978255	0.538408	C	-0.222046	2.777961	3.775506
H	-2.859956	-3.653945	0.206785	C	1.149257	2.843880	3.641578
C	-1.934845	1.165605	3.019821	C	1.528100	1.675586	2.824006
H	-2.659543	1.794024	3.522946	C	3.232933	0.162632	1.780907
C	2.864950	1.311837	2.494511	C	4.615909	-0.165051	1.443288
H	3.656900	1.998673	2.771409	C	4.593821	-1.412137	0.857724
C	-1.662273	0.838007	-3.562202	C	3.190967	-1.821982	0.805639
H	-2.002096	1.722240	-3.008329	C	2.714226	-2.984332	0.212151
H	-2.446137	0.576833	-4.286813	H	3.472742	-3.645587	-0.192259
H	-0.767254	1.125725	-4.129322	C	-2.127680	-3.036684	0.539532
C	-1.354316	-0.324375	-2.604684	H	-2.904495	-3.734039	0.241955
H	-2.272524	-0.614722	-2.069438	C	-1.978415	1.157979	2.946429
H	-0.658256	0.012524	-1.830558	H	-2.705429	1.786997	3.446508
C	-0.757417	-1.564818	-3.290082	C	2.820060	1.314296	2.449438
H	0.147221	-1.296488	-3.850579	H	3.613966	1.993618	2.740536
H	-1.464455	-2.027622	-3.993150	C	-1.279083	0.758530	-2.690847
H	-0.477280	-2.324203	-2.551689	H	-1.849055	1.365405	-1.977990
h	0.650231	-3.067979	3.854526	H	-1.847227	0.725120	-3.636854
h	1.603186	-5.302444	-1.088648	H	-0.334519	1.276345	-2.896971
h	-1.124277	-5.297727	-0.874256	C	-1.021686	-0.635381	-2.155755
h	-4.723952	-2.053155	1.080633	H	-1.917110	-1.152211	-1.793104

H	-0.357649	-0.374619	-0.958675
C	-0.065303	-1.509068	-2.938425
H	0.909251	-1.017293	-3.043390
H	-0.442872	-1.703481	-3.956875
H	0.091891	-2.478062	-2.455014
h	0.637416	-3.058335	3.795996
h	1.567638	-5.313591	-1.133844
h	-1.155008	-5.349134	-0.889207
h	-4.775888	-2.126510	1.121840
h	-4.710863	0.279121	2.609908
h	-0.931778	3.457184	4.247739
h	1.880395	3.569120	3.998695
h	5.482429	0.478442	1.595362
h	5.437758	-1.983078	0.470601

^{4}IC(III)

S	0.491044	-1.695259	3.874496
O	0.318287	0.037821	-0.045117
Fe	0.377260	-0.846093	1.540447
N	0.328193	-2.668658	0.597990
N	-1.664113	-0.896265	1.683286
N	0.443614	0.916851	2.542900
N	2.411005	-0.860717	1.446974
C	1.408268	-3.383221	0.099309
C	0.957112	-4.591137	-0.589293
C	-0.418439	-4.612755	-0.477483
C	-0.796803	-3.411834	0.258350
C	-2.526429	-1.859265	1.192220
C	-3.916471	-1.502334	1.469680
C	-3.891358	-0.315630	2.187712
C	-2.464034	0.046233	2.298973
C	-0.632570	1.580151	3.089878
C	-0.199944	2.787946	3.798877
C	1.171721	2.852422	3.668387
C	1.552525	1.674911	2.864145
C	3.260834	0.159184	1.826310
C	4.642694	-0.160575	1.473769
C	4.620974	-1.407539	0.888820
C	3.219198	-1.825133	0.854115
C	2.740244	-2.982634	0.252271
H	3.497981	-3.644028	-0.154119
C	-2.104198	-3.025692	0.550627
H	-2.881929	-3.718704	0.244980
C	-1.954272	1.162863	2.969890
H	-2.683066	1.794182	3.464935
C	2.845400	1.312783	2.490937
H	3.637977	1.997610	2.773470
C	-1.328097	0.752802	-2.953772
H	-1.804861	1.383789	-2.194313
H	-1.880010	0.907900	-3.900538
H	-0.311410	1.132753	-3.115681
C	-1.305913	-0.687523	-2.542962
H	-2.164769	-1.081216	-1.998095
H	-0.250238	-0.410956	-0.715749
C	-0.328165	-1.662550	-3.121070
H	0.654313	-1.194121	-3.258100
H	-0.642934	-2.040254	-4.112481
H	-0.198531	-2.541881	-2.480911
h	0.643998	-3.065881	3.826033
h	1.595887	-5.301388	-1.114245
h	-1.127272	-5.342742	-0.868306
h	-4.751913	-2.102661	1.109525
h	-4.688786	0.295624	2.610256
h	-0.913252	3.470716	4.260486
h	1.901761	3.581890	4.019079
h	5.506549	0.488860	1.615386
h	5.462780	-1.976574	0.494322

^{4}IC(IV)

S	0.432311	-1.711860	3.821556
O	0.287355	0.009384	-0.025424
Fe	0.396571	-0.833018	1.549469
N	0.348505	-2.647648	0.614471
N	-1.655371	-0.867910	1.688646
N	0.447820	0.901677	2.568933
N	2.417797	-0.854076	1.442796
C	1.434806	-3.373418	0.122528
C	0.967578	-4.571517	-0.564290
C	-0.409956	-4.576086	-0.464287
C	-0.788713	-3.374952	0.266348
C	-2.509340	-1.830628	1.179169
C	-3.899846	-1.470796	1.450525
C	-3.880858	-0.294258	2.184879
C	-2.457977	0.073770	2.311980
C	-0.639182	1.575870	3.103041
C	-0.197188	2.781345	3.796231
C	1.178597	2.836177	3.674894
C	1.565274	1.658277	2.883971
C	3.261403	0.173929	1.831423

C	4.638774	-0.144691	1.469103
C	4.620796	-1.394553	0.888357
C	3.224664	-1.820621	0.851372
C	2.763673	-2.990555	0.266150
H	3.521126	-3.652387	-0.135441
C	-2.097242	-2.995163	0.539484
H	-2.873036	-3.684570	0.226578
C	-1.962884	1.184712	2.984662
H	-2.688450	1.823495	3.471966
C	2.860944	1.312122	2.515736
H	3.652573	1.990418	2.810944
C	-1.274843	0.776771	-2.986423
H	-1.839418	1.393199	-2.276891
H	-1.773155	0.875130	-3.969590
H	-0.273889	1.212393	-3.096889
C	-1.199098	-0.652628	-2.544589
H	-2.069220	-1.087462	-2.051281
H	-0.285000	-0.397415	-0.723689
C	-0.141114	-1.578804	-3.061101
H	0.852023	-1.112378	-3.014319
H	-0.307640	-1.843977	-4.122605
H	-0.106494	-2.517040	-2.498866
h	0.614874	-3.078931	3.775343
h	1.600354	-5.290415	-1.084718
h	-1.120970	-5.303679	-0.855610
h	-4.733514	-2.064658	1.075834
h	-4.681640	0.304269	2.619137
h	-0.908033	3.480164	4.237159
h	1.905782	3.568212	4.026166
h	5.499981	0.510211	1.601359
h	5.464837	-1.962466	0.497031

^{4}TSreb(III)

S	0.468622	-1.685481	3.880485
O	-0.009195	-0.054256	-0.235142
Fe	0.267252	-0.827724	1.469665
N	0.235904	-2.660771	0.555491
N	-1.765635	-0.865727	1.697839
N	0.326694	0.953448	2.447882
N	2.302860	-0.848422	1.331711
C	1.304332	-3.399821	0.073167
C	0.832856	-4.589423	-0.639637
C	-0.543938	-4.560276	-0.574904
C	-0.903082	-3.354406	0.172622
C	-2.622051	-1.803025	1.156158
C	-4.013580	-1.459131	1.450238
C	-3.990339	-0.305806	2.223957
C	-2.565415	0.049484	2.353352
C	-0.723337	1.588200	3.085485
C	-0.264637	2.785914	3.787769
C	1.097271	2.872690	3.576778
C	1.447428	1.715603	2.731687
C	3.153131	0.177939	1.705807
C	4.539954	-0.165703	1.398371
C	4.520963	-1.429016	0.845461
C	3.117823	-1.836694	0.791998
C	2.638764	-3.015072	0.227632
H	3.395320	-3.690041	-0.157878
C	-2.202850	-2.943185	0.461409
H	-2.991476	-3.606725	0.121854
C	-2.044665	1.153399	3.034338
H	-2.757772	1.765147	3.574643
C	2.735325	1.348747	2.336752
H	3.528954	2.039445	2.601498
C	-1.142785	1.125982	-2.947632
H	-1.751593	1.740250	-2.271585
H	-1.659792	1.126784	-3.927807
H	-0.181891	1.632381	-3.109438
C	-0.941415	-0.260238	-2.419350
H	-1.779769	-0.738502	-1.920103
H	-0.453542	0.812435	-0.098083
C	0.136749	-1.133944	-2.967728
H	1.096735	-0.603824	-2.994015
H	-0.077647	-1.456004	-4.005582
H	0.268652	-2.034124	-2.362308
h	0.639141	-3.053428	3.817326
h	1.468536	-5.319635	-1.140404
h	-1.258088	-5.262271	-1.005323
h	-4.849567	-2.043435	1.065815
h	-4.785213	0.292440	2.669314
h	-0.957712	3.452688	4.300727
h	1.835176	3.606494	3.900961
h	5.409697	0.471673	1.557632
h	5.365634	-2.002135	0.463189

^{4}P

S	0.423301	-1.718371	3.969253
O	-0.069970	0.454497	-0.555465

Fe	0.311158	-0.908402	1.576830	h	-4.764108	0.278914	2.605672
N	0.258118	-2.645317	0.535934	h	-0.970173	3.448324	4.233460
N	-1.741639	-0.857267	1.604914	h	1.834996	3.562077	3.938989
N	0.346845	0.937249	2.422275	h	5.421375	0.474970	1.561937
N	2.316561	-0.841540	1.310033	h	5.381426	-1.989898	0.454901
C	1.342675	-3.391145	0.063994				
C	0.873132	-4.587279	-0.623787				
C	-0.505901	-4.573565	-0.548696				
C	-0.881770	-3.366345	0.172272				
C	-2.601522	-1.822497	1.102311				
C	-3.987896	-1.479150	1.403152				
C	-3.966478	-0.309446	2.152145				
C	-2.546652	0.067839	2.259840				
C	-0.725183	1.587290	3.022309				
C	-0.271772	2.772303	3.740207				
C	1.101171	2.839161	3.582676				
C	1.470936	1.685772	2.750348				
C	3.167545	0.181458	1.711594				
C	4.550984	-0.160894	1.400188				
C	4.533944	-1.418178	0.833023				
C	3.134996	-1.828898	0.767781				
C	2.674033	-3.014956	0.213663				
H	3.432695	-3.694698	-0.155239				
C	-2.188710	-2.978717	0.443819				
H	-2.967495	-3.663114	0.127447				
C	-2.047733	1.178222	2.935178				
H	-2.767336	1.795638	3.458173				
C	2.765025	1.329990	2.378769				
H	3.558895	2.004347	2.677367				
C	-1.394181	1.123816	-2.531856				
H	-2.067685	1.707101	-1.891791				
H	-1.980009	0.745197	-3.379124				
H	-0.621199	1.788987	-2.932466				
C	-0.764304	-0.040521	-1.764434				
H	-1.549745	-0.735143	-1.436149				
H	-0.624510	1.104839	-0.074169				
C	0.281642	-0.786736	-2.582035				
H	1.072436	-0.101997	-2.907046				
H	-0.182707	-1.229961	-3.471749				
H	0.739540	-1.583653	-1.992520				
h	0.613799	-3.081209	3.865678				
h	1.508242	-5.315173	-1.128636				
h	-1.213670	-5.294958	-0.957014				
h	-4.824151	-2.077158	1.041031				

Cartesian Coordinates of the Optimized $^{2}TS_{H}$(IV) from QM calculation

B3LYP/LACVP optimized $^{2}TS_{H}$(IV) of methane hydroxylation by Cpd I by Gaussian 09

S	0.593609	-1.970629	3.583028
O	0.345481	-0.130969	-0.125165
Fe	0.329135	-0.947619	1.448593
N	0.243101	-2.777669	0.601309
N	-1.665901	-0.941842	1.642255
N	0.430141	0.786736	2.465152
N	2.348114	-0.974515	1.276424
C	1.305239	-3.491070	0.061663
C	0.816603	-4.722148	-0.517956
C	-0.537360	-4.746277	-0.335320
C	-0.896113	-3.526341	0.352212
C	-2.543073	-1.956231	1.272927
C	-3.894686	-1.578686	1.616647
C	-3.834062	-0.348084	2.206874
C	-2.443682	0.043671	2.239757
C	-0.630112	1.541774	2.935837
C	-0.130911	2.745227	3.563879
C	1.230850	2.714611	3.465296
C	1.582573	1.494955	2.771515
C	3.225615	-0.009587	1.735342
C	4.579815	-0.370030	1.369374
C	4.511271	-1.552740	0.691301
C	3.114581	-1.933123	0.639219
C	2.634897	-3.101321	0.069775
H	3.354672	-3.767179	-0.393315
C	-2.192242	-3.153804	0.673842
H	-2.989798	-3.847542	0.432015
C	-1.970221	1.205150	2.825750
H	-2.697954	1.887107	3.251154
C	2.876713	1.130618	2.439720
H	3.676760	1.796217	2.744383
C	-1.757933	0.447187	-1.407203
H	-0.623910	0.110081	-0.662313
H	-1.297600	0.854525	-2.305164
H	-2.259904	-0.510170	-1.526605
H	-2.264259	1.167290	-0.768576
H	0.976865	-3.223353	3.144674
H	1.441027	-5.459723	-1.000701
H	-1.241863	-5.506498	-0.639697
H	-4.765016	-2.191501	1.432269
H	-4.644726	0.245320	2.603966
H	-0.754230	3.502916	4.015754
H	1.945407	3.443803	3.818078
H	5.454552	0.216675	1.608920
H	5.318669	-2.130315	0.265380

B3LYP/def2-TZVP optimized $^{2}TS_{H}$(IV) of methane hydroxylation by Cpd I by Turbomole 6.3.1

S	0.6064202	-1.9314321	3.5455039
O	0.3676029	-0.1542656	-0.1194257
Fe	0.3294983	-0.9640566	1.4487307
N	0.2481427	-2.7892167	0.6004909
N	-1.6635724	-0.9589570	1.6383437
N	0.4330553	0.7804677	2.4527578
N	2.3518764	-0.9702843	1.2539589
C	1.3032804	-3.5019197	0.0981676
C	0.8274925	-4.7297210	-0.4786253
C	-0.5206443	-4.7412146	-0.3290716
C	-0.8765669	-3.5189257	0.3381106
C	-2.5264261	-1.9511126	1.2530906
C	-3.8725636	-1.5873853	1.5997065
C	-3.8105223	-0.3797396	2.2134550
C	-2.4258755	0.0027841	2.2477967
C	-0.6159987	1.5101158	2.9337069
C	-0.1306252	2.7180694	3.5433051
C	1.2194155	2.7088152	3.4140828
C	1.5668331	1.4962874	2.7242513
C	3.2117591	-0.0049346	1.6873811
C	4.5628744	-0.3656475	1.3418184
C	4.4997007	-1.5592806	0.7040674
C	3.1095071	-1.9346511	0.6588057
C	2.6309183	-3.1143416	0.1194299
H	3.3522018	-3.7912502	-0.3186731
C	-2.1716614	-3.1391139	0.6435202
H	-2.9672641	-3.8264621	0.3886028
C	-1.9505221	1.1560821	2.8418925
H	-2.6767625	1.8270883	3.2805923
C	2.8566632	1.1404121	2.3752364

H	3.6517960	1.8157383	2.6618355
C	-1.7156691	0.5060438	-1.3288237
H	-0.6713123	0.1409290	-0.6552292
H	-1.2780932	0.9656096	-2.2100120
H	-2.2534533	-0.4157160	-1.5266807
H	-2.2392060	1.1980459	-0.6771872
H	0.7482032	-3.2091417	3.1544389
H	1.4583654	-5.4732890	-0.9401439
H	-1.2253051	-5.4957316	-0.6420183
H	-4.7407910	-2.1965719	1.4020565
H	-4.6171663	0.2071358	2.6244150
H	-0.7567947	3.4668128	4.0028255
H	1.9308005	3.4492870	3.7448462
H	5.4332758	0.2292336	1.5707054
H	5.3072462	-2.1496889	0.3002147

B3LYP/LACVP optimized $^{2}TS_{H}$(IV) of *i*-propane hydroxylation by Cpd I by Gaussian 09

S	0.676922	-1.976153	3.609458
O	-0.065300	0.147813	0.152408
Fe	0.325706	-0.859665	1.531120
N	0.985505	-2.440595	0.499436
N	-1.512101	-1.674609	1.599791
N	-0.328211	0.729259	2.614694
N	2.208126	-0.131272	1.631709
C	2.297801	-2.698459	0.118826
C	2.360069	-3.954429	-0.593497
C	1.092733	-4.462936	-0.628973
C	0.236524	-3.527741	0.064778
C	-1.925064	-2.856690	1.009733
C	-3.335738	-3.058913	1.256101
C	-3.771385	-1.993765	1.991581
C	-2.634259	-1.124455	2.201433
C	-1.621269	0.946457	3.054175
C	-1.693208	2.217785	3.744952
C	-0.440771	2.759784	3.720251
C	0.414112	1.824865	3.017400
C	2.601464	1.081571	2.180428
C	4.022574	1.264451	1.983709
C	4.481458	0.169326	1.307888
C	3.345590	-0.695839	1.079169
C	3.392717	-1.892862	0.380748
H	4.357833	-2.221900	0.011600
C	-1.116389	-3.719662	0.286986
H	-1.570443	-4.618501	-0.115101
C	-2.690553	0.085354	2.873725
H	-3.649033	0.384008	3.283808
C	1.774512	1.992947	2.817983
H	2.229194	2.902111	3.195823
C	-1.117422	-0.003917	-2.868882
H	-1.979457	-0.512083	-2.424628
H	-1.139098	-0.189934	-3.954308
H	-1.237617	1.074222	-2.713718
C	0.188515	-0.499304	-2.273081
H	0.280847	-1.590987	-2.283103
H	0.090697	-0.256773	-1.045359
C	1.452041	0.211445	-2.723929
H	1.368487	1.294516	-2.578154
H	1.631426	0.031850	-3.795705
H	2.329807	-0.143244	-2.173912
H	1.745765	-1.221719	4.052242
H	3.265781	-4.382616	-0.997645
H	0.754892	-5.391255	-1.066108
H	-3.902056	-3.909543	0.905937
H	-4.766787	-1.796854	2.362029
H	-2.591838	2.623927	4.185797
H	-0.107192	3.698541	4.137846
H	4.579884	2.126121	2.321317
H	5.488921	-0.044254	0.981789

B3LYP/def2-TZVP optimized $^{2}TS_{H}$(IV) of *i*-propane hydroxylation by Cpd I by Turbomole 6.3.1

S	0.6405462	-1.9550598	3.5880764
O	-0.0459914	0.1522433	0.1830637
Fe	0.3412903	-0.8564214	1.5528531
N	0.9973755	-2.4323056	0.5100329
N	-1.5069309	-1.6580364	1.6040463
N	-0.3224211	0.7458361	2.6138292
N	2.2205638	-0.1350688	1.6579811
C	2.2898798	-2.6830444	0.1317924
C	2.3548921	-3.9278573	-0.5832553
C	1.0958887	-4.4308155	-0.6170476
C	0.2530578	-3.4983458	0.0799163
C	-1.9112602	-2.8211613	1.0148910
C	-3.3197351	-3.0132091	1.2299931
C	-3.7566273	-1.9473632	1.9457830

C	-2.6188750	-1.0975088	2.1701986	N	-1.752846	-1.093377	1.527318
C	-1.6024923	0.9686303	3.0276773	N	0.348646	0.727571	2.085049
C	-1.6758944	2.2275482	3.7239391	N	2.269999	-1.259893	1.334741
C	-0.4256804	2.7498671	3.7244004	C	1.213920	-3.942230	0.568743
C	0.4188212	1.8112413	3.0305804	C	0.718541	-5.252721	0.210278
C	2.6086475	1.0523848	2.2160708	C	-0.641365	-5.220368	0.339326
C	4.0233158	1.2344534	2.0336265	C	-0.996143	-3.887132	0.771880
C	4.4765062	0.1534221	1.3513944	C	-2.638373	-2.145424	1.317785
C	3.3401988	-0.6937414	1.1110938	C	-3.993303	-1.689274	1.528372
C	3.3822086	-1.8818934	0.4033415	C	-3.927216	-0.370668	1.878842
H	4.3448107	-2.2096659	0.0341945	C	-2.530211	-0.000860	1.894451
C	-1.0985317	-3.6833017	0.3004161	C	-0.709777	1.575137	2.362434
H	-1.5526867	-4.5767162	-0.1066238	C	-0.205731	2.866667	2.774575
C	-2.6721796	0.1154180	2.8322022	C	1.157665	2.794731	2.741762
H	-3.6324536	0.4239963	3.2234016	C	1.505689	1.460508	2.304033
C	1.7814567	1.9614338	2.8509922	C	3.151615	-0.240799	1.643635
H	2.2396311	2.8603744	3.2414253	C	4.510283	-0.685707	1.410337
C	-1.1443084	-0.1319134	-2.8293765	C	4.439908	-1.972863	0.961324
H	-1.9516924	-0.7047628	-2.3705746	C	3.037433	-2.333350	0.920435
H	-1.1728045	-0.3198160	-3.9096405	C	2.551410	-3.579457	0.559458
H	-1.3494876	0.9294031	-2.6728922	H	3.272121	-4.332319	0.259787
C	0.2039759	-0.5167719	-2.2621457	C	-2.293898	-3.439091	0.966459
H	0.3794857	-1.5939704	-2.2997504	H	-3.098420	-4.152605	0.826638
H	0.1324002	-0.2935622	-1.0727157	C	-2.052483	1.244462	2.265845
C	1.3841084	0.2791718	-2.7734525	H	-2.779416	2.006092	2.525043
H	1.2388279	1.3494216	-2.6099517	C	2.802538	1.017839	2.104533
H	1.5118963	0.1232296	-3.8516821	H	3.606015	1.715340	2.314051
H	2.3123107	-0.0175584	-2.2830360	C	-1.627414	-0.177849	-1.730285
H	1.8012834	-1.3855108	3.9532175	H	-0.634049	-0.462312	-0.909518
H	3.2590052	-4.3528516	-0.9906063	H	-2.166709	-1.126929	-1.766127
H	0.7530327	-5.3542621	-1.0571761	H	-2.166175	0.592882	-1.175256
H	-3.8853377	-3.8579951	0.8689731	C	-0.972030	0.263502	-3.016101
H	-4.7556626	-1.7356331	2.2936480	H	-1.733451	0.522931	-3.769425
H	-2.5762147	2.6385091	4.1533404	H	-0.346225	-0.528888	-3.439903
H	-0.0852262	3.6788016	4.1545399	H	-0.345437	1.148447	-2.863144
H	4.5800146	2.0895310	2.3841638	H	0.863606	-3.072256	3.532338
H	5.4817717	-0.0633615	1.0253884	H	1.343122	-6.077831	-0.099789
				H	-1.351705	-6.013030	0.154825
B3LYP/LACVP optimized ^2TS_H(IV) of ethane hydroxylation by Cpd I by Gaussian 09				H	-4.869720	-2.312526	1.426191
				H	-4.738695	0.299303	2.123074
S	0.411077	-1.779505	3.709886	H	-0.827188	3.705911	3.050904
O	0.353771	-0.680421	-0.277057	H	1.875798	3.564671	2.983189
Fe	0.244823	-1.167804	1.414252	H	5.388792	-0.079137	1.575057
N	0.149752	-3.123801	0.921352	H	5.249530	-2.632936	0.686122